# Electronic Supplementary Information

# Construction of isoxazolone-fused phenanthridines *via* Rh-catalyzed Cascade C-H Activation/Cyclization of 3-Arylisoxazolones with Cyclic 2-Diazo-1,3-diketones

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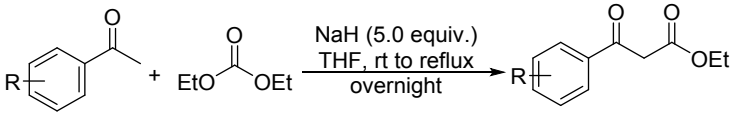
## Table of contents

**1. General comments**

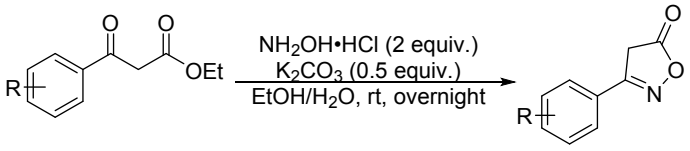
Unless otherwise specified, all reagents and starting materials were purchased from commercial sources and used as received without purification. The solvents were purified and dried using standard procedures. The chromatography solvents were technical grade and distilled prior to use. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. The $^{1}H$ and $^{13}C$ NMR spectra were recorded on a 500 MHz and 125 MHz NMR spectrometers, unless otherwise specified. Chemical shifts ($\delta$) in parts per million were reported relative to the residual signals of chloroform (7.26 ppm for $^{1}H$ and 77.0 ppm for $^{13}C$), and all $^{13}C$ NMR were recorded with proton broadband decoupling and indicated as $^{13}C\{1H\}$ NMR. Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), or m (multiplet), and the coupling constants (*J*) are reported in Hertz (Hz). HRMS analysis with a quadrupole time-of-flight (TOF) mass spectrometer yielded ion mass/charge (*m/z*) ratios in atomic mass units. The melting points were measured using SGWX-4 melting point apparatus.

**2. General procedure for the synthesis of ethyl 3-oxo-3-arylpropanoate.**



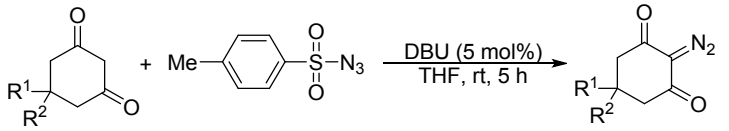

To a suspension of sodium hydride (60% in mineral oil, 5 equiv) and diethyl carbonate (10 mmol, 2.0 equiv.) in THF (10 mL) was added a solution of substituted acetophenone (5 mmol, 1.0 equiv.) in THF (10 mL) dropwise under reflux. The mixture was refluxed overnight then quenched with $H_2O$. The mixture was extracted with ethyl acetate for 3 times, and the combined organic phase was washed with brine, dried with anhydrous $Na_2SO_4$, and concentrated under reduced pressure. The residue was purified on a silica gel column to afford substituted ethyl benzoylacetate (petroleum ether /ethyl acetate, 20:1, v/v).

**3. General procedure for the synthesis of 3-aryl-5-isoxazolones.**



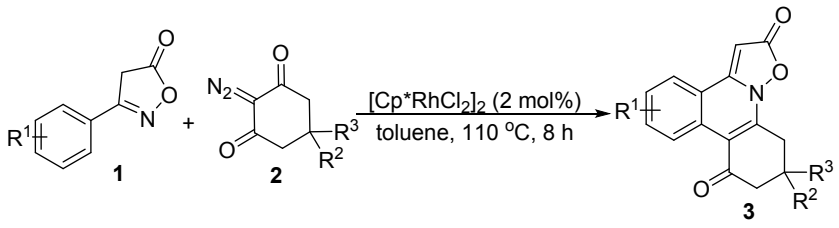

To a mixture of ethyl benzoylacetate (3 mmol, 1.0 equiv.), hydroxylamine hydrochloride (6 mmol, 2.0 equiv.) and potassium carbonate (1.5 mmol, 0.5 equiv.) in ethanol/water (10 mL, v/v = 1:1) was stirred at room temperature overnight. The solid was filtered, washed with water and extracted three times with ether. The combined organic layers were dried over $Na_2SO_4$, and concentrated under reduced pressure. The residue was purified on a silica gel column to afford substituted 3-arylisoxazol-5-ones (petroleum ether /ethyl acetate, 3:1, v/v).

**4. General procedure for the synthesis of 2-diazo-1,3-diketones.**



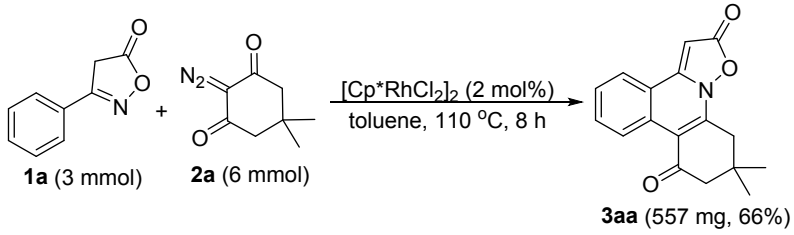
A mixture of 1,3-diketones (1 mmol), 4-methylbenzenesulfonyl azide (1 mmol), and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (5 mol%) in tetrahydrofuran (THF) (3 mL) in a sealed tube was stirred at room temperature for 5 h under argon atmosphere. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, extracted with $CH_2Cl_2$ (3 × 10 mL), and washed with brine. The organic layers were combined, dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:3, v/v) as the elution solvent to give desired 2-diazo-1,3-diketones.

**5. General procedure for the synthesis of isoxazolo[2,3-*f*]phenanthridines.**



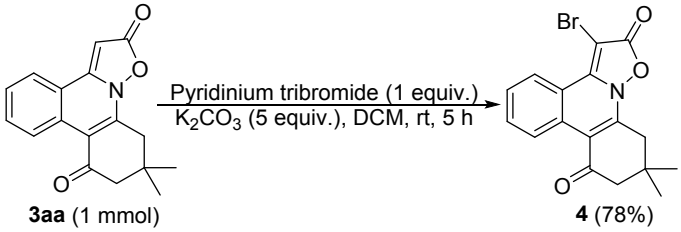

A mixture of 3-arylisoxazol-5(4*H*)-ones **1** (0.25 mmol), cyclic 2-diazo-1,3-diketones **2** (0.5 mmol), and $[Cp^*RhCl_2]_2$ (0.005 mmol) in toluene (4 mL) in a sealed tube was heated to 110 ºC in an oil bath for 8 h under air atmosphere. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, extracted with $CH_2Cl_2$ (3 × 10 mL), and washed with brine. The organic layers were combined, dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:4, v/v) as the elution solvent to give desired product **3**.

**6. Large-scale synthesis.**




A mixture of 3-phenylisoxazol-5(4*H*)-one **1a** (3 mmol), 2-diazo-5,5-dimethylcyclohexane-1,3-dione **2a** (6 mmol), and $[Cp^*RhCl_2]_2$ (0.06 mmol) in toluene (15 mL) in a sealed tube was heated to 110 ºC in an oil bath for 8 h under air atmosphere. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, extracted with $CH_2Cl_2$ (3 × 20 mL), and washed with brine. The organic layers were combined, dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:4, v/v) as the elution solvent to give desired product **3aa** in 66% yield (557 mg).

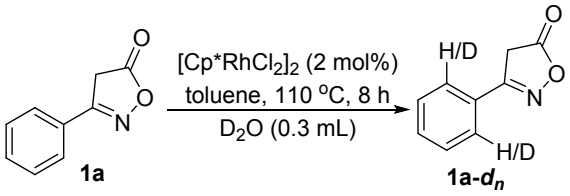
**7. General procedure for further transformation.**



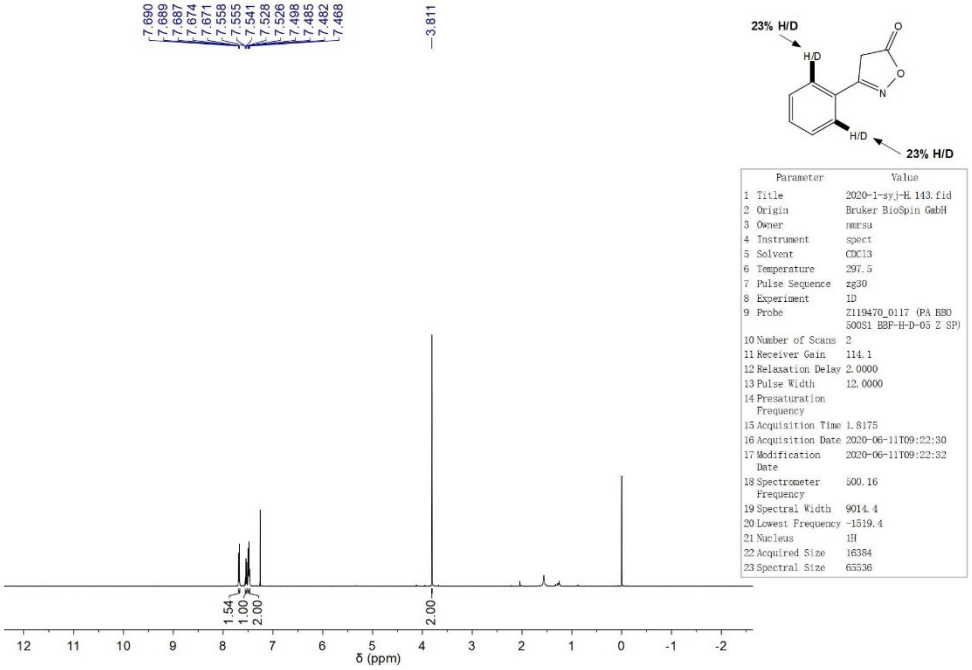

Compound **3aa** (1.0 mmol) was dissolved in dichloromethane (5 mL). Then potassium carbonate (5.0 mmol) and pyridinium tribromide (1.0 mmol) were added to this mixture at room temperature. The reaction mixture was stirred at room temperature for 5 h and then quenched with a saturated aqueous sodium bicarbonate solution (10 mL). The organic phase was extracted with ethyl acetate (3 × 20 mL), dried over $Na_2SO_4$, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:8, v/v) as the elution solvent to give compound **4** in 78% yield.

**8. H/D exchange experiments.**

(1) H/D exchange experiments of substrate **1a**.




To the mixture of 3-phenylisoxazol-5(4*H*)-one **1a** (0.25 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol) and toluene (3 mL) in a sealed tube was added $D_2O$ (0.3 mL) at room temperature under air atmosphere. The stirred mixture was then heated to 110 °C in an oil bath for further 2 h. After being cooled down to room temperature, it was purified by preparative chromatography to afford the starting material, which was subject to $^1$H NMR test to determine the ratio of **1a** and **1a-*d*$_n$**.

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| 16 Acquisition Date | 2020-06-11T09:22:30 |
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| 19 Spectral Width | 9014.4 |
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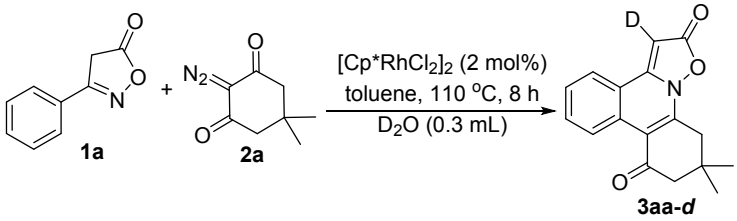
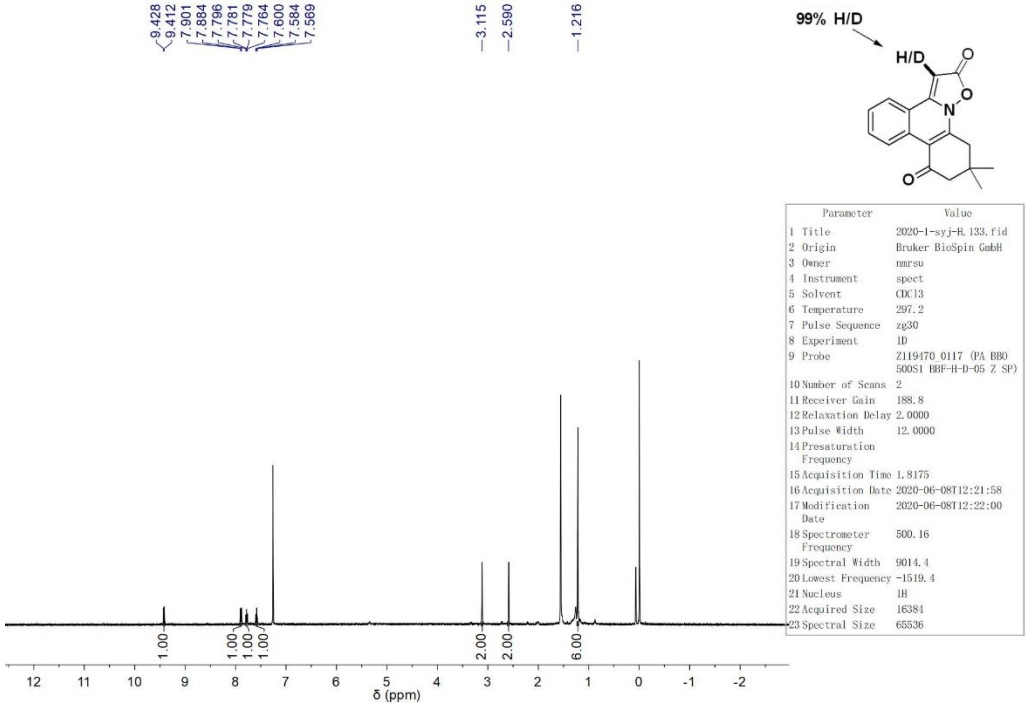
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

(2) H/D exchange experiments of compound **3aa**.




To the mixture of 3-phenylisoxazol-5(4*H*)-one **1a** (0.25 mmol), 2-diazo-5,5-dimethylcyclohexane-1,3-dione **2a** (0.5 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol), and toluene (4 mL) in a sealed tube was added $D_2O$ (0.3 mL) at room temperature under air atmosphere. The stirred mixture was then heated to 110 ºC in an oil bath for 8 h. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, extracted with $CH_2Cl_2$ (3 × 10 mL), and washed with brine. The organic layers were combined, dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:4, v/v) as the elution solvent to give desired product **3aa-*d*** in 64% yield.

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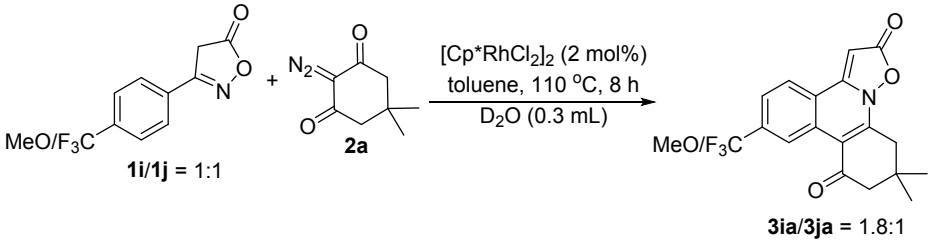
| 23 Spectral Size | 65536 |

**9. General procedure for competitive experiment.**

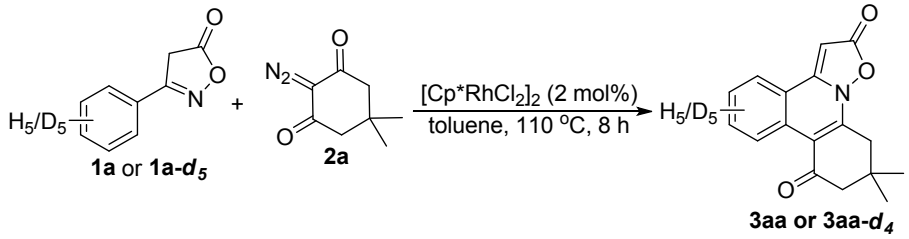



A mixture of 3-(4-methoxyphenyl)isoxazol-5(4*H*)-one **1i** (0.1 mmol), 3-(4-(trifluoromethyl)phenyl)isoxazol-5(4*H*)-one **1j** (0.1 mmol), 2-diazo-5,5-dimethylcyclohexane-1,3-dione **2a** (0.2 mmol), and $[Cp^*RhCl_2]_2$ (0.002 mmol) in toluene (4 mL) in a sealed tube was heated

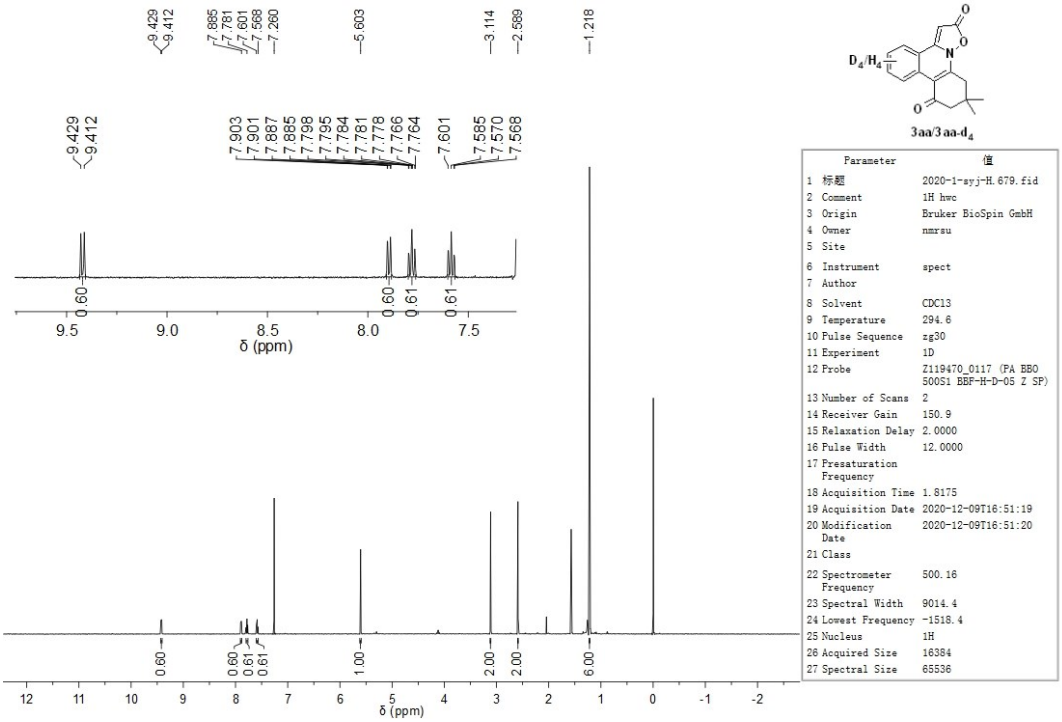
to 110 ºC in an oil bath for 8 h under air atmosphere. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, extracted with $CH_2Cl_2$ (3 × 10 mL), and washed with brine. The organic layers were combined, dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:4, v/v) as the elution solvent to give desired product **3ia** and **3ja** in 52% and 29%, respectively.

**10. Kinetic Isotope Effect studies.**

(1) Parallel experiments




To the mixture of 3-phenylisoxazol-5(4*H*)-one **1a** (0.1 mmol) or 3-phenylisoxazol-5(4*H*)-one **1a-*d*$_5$** (0.1 mmol), 2-diazo-5,5-dimethylcyclohexane-1,3-dione **2a** (0.2 mmol), $[Cp^*RhCl_2]_2$ (0.002 mmol), and toluene (1.5 mL) in a sealed tube at room temperature under air atmosphere. The stirred mixture was then heated to 110 ºC in an oil bath for 2 h. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, combined, extracted with $CH_2Cl_2$ (3 × 10 mL), and washed with brine. The organic layer was dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residues were combined and purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:4, v/v) as the elution solvent to afford the mixed products **3aa** and **3aa-*d*$_4$**. The $\mathbf{K_{H/D}}$ value was determined to be 1.5 by the $^1$H NMR test.

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| 5 Site | |
| 6 Instrument | spect |
| 7 Author | |
| 8 Solvent | CDCl3 |
| 9 Temperature | 294.6 |
| 10 Pulse Sequence | zg30 |
| 11 Experiment | 1D |
| 12 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
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| 14 Receiver Gain | 150.9 |
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| 16 Pulse Width | 12.0000 |
| 17 Presaturation Frequency | |
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| 23 Spectral Width | 9014.4 |
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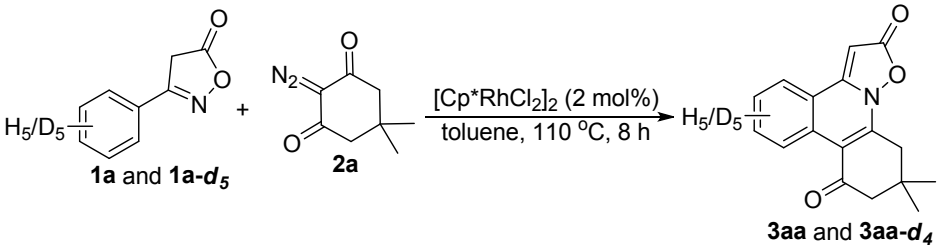
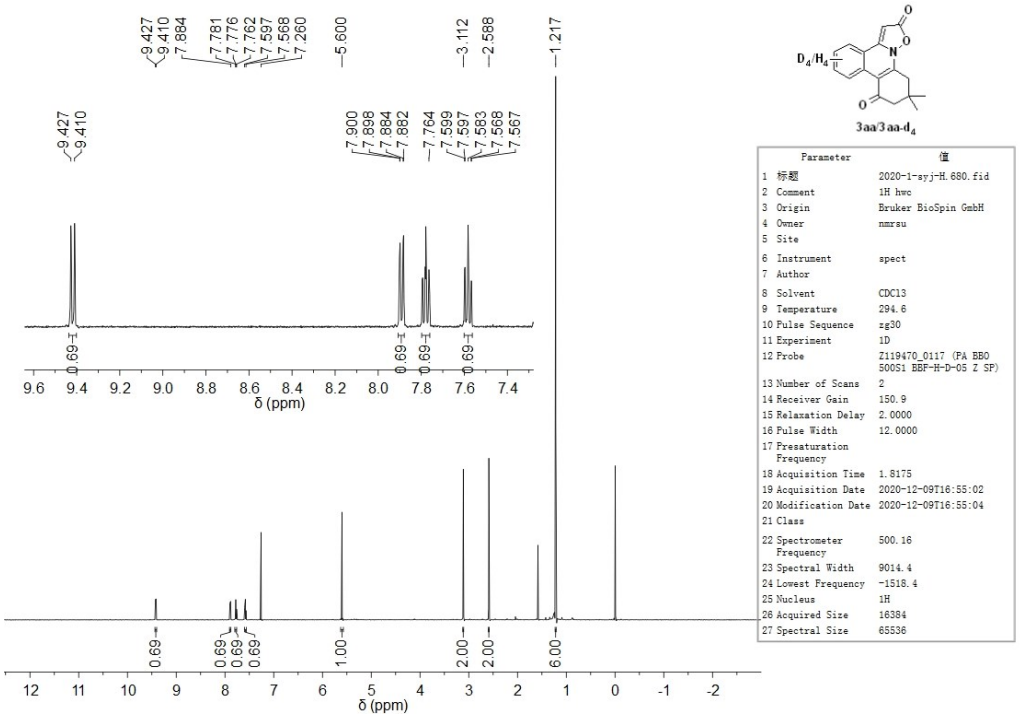
| 25 Nucleus | 1H |
| 26 Acquired Size | 16384 |
| 27 Spectral Size | 65536 |

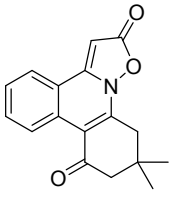
(2) competitive reaction



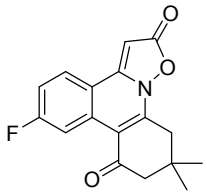

To the mixture of 3-phenylisoxazol-5(4*H*)-one **1a** (0.25 mmol), 3-phenylisoxazol-5(4*H*)-one **1a-*d*$_5$** (0.25 mmol), 2-diazo-5,5-dimethylcyclohexane-1,3-dione **2a** (0.5 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol), and toluene (4 mL) in a sealed tube at room temperature under air atmosphere. The stirred mixture was then heated to 110 ºC in an oil bath for 2 h. After the reaction was complete (as determined using TLC), the reaction mixture was cooled to room temperature, extracted with $CH_2Cl_2$ (3 × 10 mL), and washed with brine. The organic layers were combined, dried over $Na_2SO_4$, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:4, v/v) as the elution solvent to afford the product **3aa** and **3aa-*d*$_4$**. The $\mathbf{K_{H/D}}$ value was determined to be 2.2 by the $^1$H NMR test.



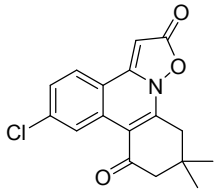

## 11. Characterization data for all compounds



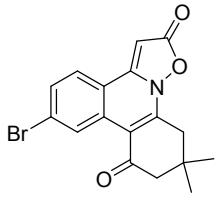
***10,10-Dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione (3aa)***. The title compound was prepared from 3-phenylisoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 72% yield (50 mg); mp = 205–206 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.42 (d, $J$ = 8.6 Hz, 1H), 7.91–7.88 (m, 1H), 7.80–7.76 (m, 1H), 7.60–7.57 (m, 1H), 5.60 (s, 1H), 3.11 (s, 2H), 2.59 (s, 2H), 1.22 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.99, 168.02, 152.44, 143.56, 133.43, 129.72, 128.04, 127.21, 125.82, 119.78, 109.31, 75.89, 52.97, 37.72, 32.36, 28.35; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{16}NO_3$ 282.1125; found 282.1132.



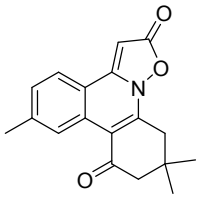

***6-Fluoro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3ba).** The title compound was prepared from 3-(4-fluorophenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 53% yield (39 mg); mp = 205–206 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.20 (dd, $J$ = 12.0, 2.6 Hz, 1H), 7.90 (dd, $J$ = 8.9, 5.7 Hz, 1H), 7.34–7.30 (m, 1H), 5.57 (s, 1H), 3.11 (s, 2H), 2.59 (s, 2H), 1.22 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.66, 167.74, 166.70 (d, $J_{C\text{-}F}$ = 251.7 Hz), 151.91, 144.40, 132.14 (d, $J_{C\text{-}F}$ = 11.8 Hz), 128.34 (d, $J_{C\text{-}F}$ = 10.0 Hz), 117.08 (d, $J_{C\text{-}F}$ = 24.5 Hz), 116.37, 113.27 (d, $J_{C\text{-}F}$ = 26.0 Hz), 108.54, 108.51, 75.92, 52.75, 37.74, 32.31, 28.33; $^{19}$F NMR (471 MHz, $CDCl_3$) $\delta$ -102.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}FNO_3$ 300.1030; found 300.1025.



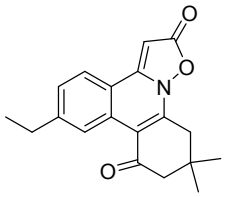

***6-Chloro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*****(3ca).** The title compound was prepared from 3-(4-chlorophenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 57% yield (45 mg); mp = 229- 30 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.51 (d, $J$ = 2.0 Hz, 1H), 7.82 (d, $J$ = 8.6 Hz, 1H), 7.55 (dd, $J$ = 8.6, 2.0 Hz, 1H), 5.60 (s, 1H), 3.11 (s, 2H), 2.59 (s, 2H), 1.22 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.56, 167.66, 151.95, 144.44, 131.46, 130.95, 129.97, 128.93, 127.02, 118.39, 108.12, 76.40, 52.80, 37.78, 32.33, 28.33; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}ClNO_3$ 316.0735; found 316.0740.



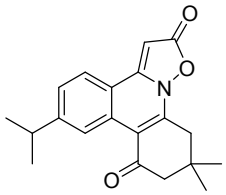
***6-Bromo-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*(3da).** The title compound was prepared from 3-(4-bromophenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a red solid in 78% yield (69 mg); mp = 217-218 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.67 (d, $J$ = 1.8 Hz, 1H), 7.75–7.72 (m, 1H), 7.70–7.67 (m, 1H), 5.60 (s, 1H), 3.11 (s, 2H), 2.58 (s, 2H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.56, 167.61, 151.82, 144.43, 131.34, 130.85, 129.81, 128.82, 126.96, 118.28, 108.01, 76.33, 52.72, 37.69, 32.26, 28.28; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}BrNO_3$ 360.0230; found 360.0239.



***6,10,10-Trimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (3ea).** The title compound was prepared from 3-(*p*-tolyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 76% yield (56 mg); mp = 200-201 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.24 (s, 1H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.41 (d, $J$ = 8.2 Hz, 1H), 5.55 (s, 1H), 3.10 (s, 2H), 2.58 (s, 2H), 2.56 (s, 3H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.18, 168.21, 152.37, 144.49, 143.54, 129.73, 129.53, 126.85, 125.71, 117.51, 109.14, 75.26, 53.01, 37.71, 32.32, 28.31, 22.60; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}NO_3$ 296.1281; found 296.1285.

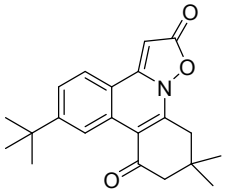


***6-Ethyl-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (3fa).** The title compound was prepared from 3-(4-ethylphenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 73% yield (56 mg); mp = 171-172 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.27 – 9.26 (m, 1H), 7.81 (d, $J$ = 8.2 Hz, 1H), 7.43 (dd, $J$ = 8.2, 1.7 Hz, 1H), 5.54 (s, 1H), 3.10 (s, 2H), 2.84 (q, $J$ = 7.6 Hz, 2H), 2.58 (s, 2H), 1.32 (t, $J$ = 7.6 Hz, 3H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.06, 167.99, 152.19, 150.46, 143.44, 129.72, 128.30, 125.73, 125.62, 117.55, 109.03, 75.10, 52.88, 37.54, 32.17, 29.69, 28.21, 15.34; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{20}NO_3$ 310.1438; found 310.1434.



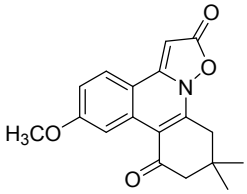
***6-isopropyl-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***

**(3ga).** The title compound was prepared from 3-(4-isopropylphenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 71% yield (57 mg); mp = 105-106 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.30 (d, $J$ = 1.6 Hz, 1H), 7.81 (d, $J$ = 8.3 Hz, 1H), 7.46 (dd, $J$ = 8.3, 1.6 Hz, 1H), 5.53 (s, 1H), 3.13–3.08 (m, 3H), 2.57 (s, 2H), 1.33 (d, $J$ = 6.9 Hz, 6H), 1.20 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.20, 168.19, 155.17, 152.37, 143.49, 129.94, 127.02, 125.91, 124.59, 117.86, 109.31, 75.23, 53.07, 37.72, 35.04, 32.33, 28.32, 23.82; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{22}NO_3$ 324.1594; found 324.1587



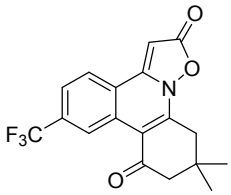
***6-(tert-Butyl)-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***

**(3ha).** The title compound was prepared from 3-(4-(*tert*-butyl)phenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 83% yield (69 mg); mp = 136-137 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.51 (d, $J$ = 1.7 Hz, 1H), 7.82 (d, $J$ = 8.5 Hz, 1H), 7.65 (dd, $J$ = 8.5, 1.9 Hz, 1H), 5.55 (s, 1H), 3.10 (s, 2H), 2.58 (s, 2H), 1.42 (s, 9H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.27, 168.23, 157.41, 152.31, 143.51, 129.75, 126.15, 125.56, 123.40, 117.49, 109.46, 75.26, 53.14, 37.78, 35.88, 32.37, 31.24, 28.35; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{24}NO_3$ 338.1751; found 338.1750.



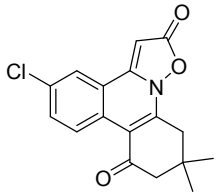
***6-Methoxy-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***

**(3ia).** The title compound was prepared from 3-(4-methoxyphenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 3:1, $R_f$ = 0.5) to afford a yellow solid in 82% yield (64 mg); mp = 192-193 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.00 (d, $J$ = 2.4 Hz, 1H), 7.80–7.75 (m, 1H), 7.18–7.13 (m, 1H), 5.47 (s, 1H), 3.98 (s, 3H), 3.10 (s, 2H), 2.58 (s, 2H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.19, 168.22, 152.38, 144.49, 143.54, 129.73, 129.53, 126.86, 125.71, 117.52, 109.14, 75.26, 53.01, 37.71, 32.32, 28.31, 22.60; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}NO_4$ 312.1230; found 312.1237.

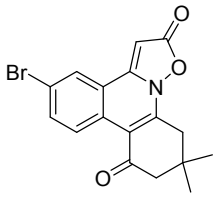


***10,10-Dimethyl-6-(trifluoromethyl)-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-***

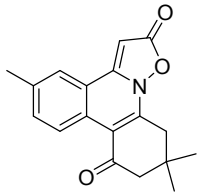
***dione* (3ja).** The title compound was prepared from 3-(4-(trifluoromethyl)phenyl)isoxazol-5(*4H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 73% yield (63 mg); mp = 206-207 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.81 (s, 1H), 8.00 (d, $J$ = 8.4 Hz, 1H), 7.78 (dd, $J$ = 8.4, 1.4 Hz, 1H), 5.69 (s, 1H), 3.13 (s, 2H), 2.61 (s, 2H), 1.23 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.58, 167.34, 151.46, 144.72, 135.03 (q, $J_{C\text{-}F}$ = 32.6 Hz), 129.82, 126.56, 124.65 (q, $J_{C\text{-}F}$ = 4.3 Hz), 124.08 (q, $J_{C\text{-}F}$ = 3.1 Hz), 122.43, 121.72, 108.52, 77.38, 52.63, 37.60, 32.25, 28.19; $^{19}$F NMR (471 MHz, $CDCl_3$) $\delta$ -63.1; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{15}F_3NO_3$ 350.0999; found 350.0994.




***5-chloro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (3ka).** The title compound was prepared from 3-(3-chlorophenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 52% yield (40 mg); mp = 216-217 ºC; $^1$H NMR (500 MHz, C $CDCl_3$ $\delta$ 9.40 (d, $J$ = 9.1 Hz, 1H), 7.85 (d, $J$ = 2.2 Hz, 1H), 7.71 (dd, $J$ = 9.1, 2.2 Hz, 1H), 5.60 (s, 1H), 3.10 (s, 2H), 2.58 (s, 2H), 1.22 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.78, 167.61, 151.33, 143.75, 134.00, 133.71, 128.95, 128.12, 124.98, 120.97, 108.78, 76.52, 52.81, 37.67, 32.34, 28.32; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}ClNO_3$ 316.0735; found 316.0737.

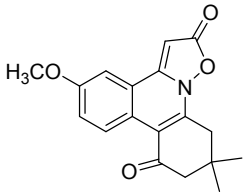



***5-bromo-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (3la).** The title compound was prepared from 3-(3-bromophenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 54% yield (48 mg); mp = 217-218 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.32 (d, $J$ = 9.1 Hz, 1H), 8.00 (d, $J$ = 2.1 Hz, 1H), 7.84 (dd, $J$ = 9.1, 2.2 Hz, 1H), 5.60 (s, 1H), 3.09 (s, 2H), 2.58 (s, 2H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.76, 167.60, 151.23, 143.88, 136.51, 129.04, 128.50, 128.14, 121.97, 121.30, 108.84, 76.57, 52.86, 37.74, 32.37, 28.35; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}BrNO_3$ 360.0230; found 360.0238.

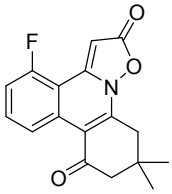



***5,10,10-Trimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (3ma).** The title compound was prepared from 3-(*m*-tolyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-

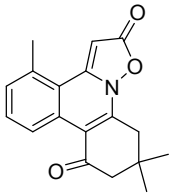
dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 74% yield (54 mg); mp = 229-230 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.27 (d, $J$ = 8.7 Hz, 1H), 7.65–7.62 (m, 1H), 7.58 (dd, $J$ = 8.6, 1.7 Hz, 1H), 5.54 (s, 1H), 3.08 (s, 2H), 2.56 (s, 2H), 2.51 (s, 3H), 1.20 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.10, 168.20, 152.31, 142.79, 138.39, 135.04, 127.36, 127.03, 125.37, 119.88, 109.40, 75.49, 52.95, 37.62, 32.38, 28.35, 21.41; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}NO_3$ 296.1281; found 296.1275.



***5-Methoxy-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3na).** The title compound was prepared from 3-(3-methoxyphenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 3:1, $R_f$ = 0.5) to afford a yellow solid in 70% yield (54 mg); mp = 209-210 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.36 (d, $J$ = 9.4 Hz, 1H), 7.37 (dd, $J$ = 9.4, 2.8 Hz, 1H), 7.18 (d, $J$ = 2.8 Hz, 1H), 5.53 (s, 1H), 3.94 (s, 3H), 3.09 (s, 2H), 2.57 (s, 2H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.18, 168.21, 152.37, 144.49, 143.54, 129.73, 129.53, 126.85, 125.71, 117.51, 109.14, 75.26, 53.01, 37.71, 32.32, 28.31, 22.60; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}NO_4$ 312.1230; found 312.1235.

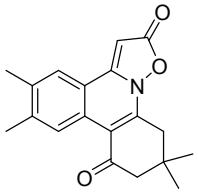


***4-Fluoro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3oa).** The title compound was prepared from 3-(2-fluorophenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 68% yield (50 mg); mp = 192-193 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.20 (d, $J$ = 8.6 Hz, 1H), 7.73–7.68 (m, 1H), 7.26–7.23 (m, 1H), 5.82 (d, $J$ = 4.4 Hz, 1H), 3.10 (s, 2H), 2.57 (s, 2H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.57, 167.88 (d, $J_{C\text{-}F}$ = 3.0 Hz ), 161.21 (d, $J_{C\text{-}F}$ = 254.7 Hz ), 147.90, 144.56, 134.18, 131.48, 122.65 (d, $J_{C\text{-}F}$ = 3.7 Hz ), 113.80 (d, $J_{C\text{-}F}$ = 19.2 Hz ), 110.26 (d, $J_{C\text{-}F}$ = 13.3 Hz ), 108.39, 81.33 (d, $J_{C\text{-}F}$ = 13.6 Hz ), 52.83, 37.81, 32.23, 28.32; $^{19}$F NMR (471 MHz, $CDCl_3$) $\delta$ -110.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}FNO_3$ 300.1030; found 300.1029.

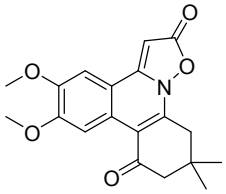


***4,10,10-Trimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3pa).** The

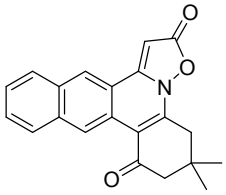
title compound was prepared from 3-(*o*-tolyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 72% yield (52 mg); mp = 217-218 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.32 (d, $J$ = 8.6 Hz, 1H), 7.65–7.60 (m, 1H), 7.37 (d, $J$ = 7.3 Hz, 1H), 5.75 (s, 1H), 3.09 (s, 2H), 2.71 (s, 3H), 2.57 (s, 2H), 1.20 (s, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) $\delta$ 195.82, 167.77, 151.30, 143.51, 137.74, 132.65, 131.05, 130.66, 124.74, 120.03, 109.50, 81.41, 53.11, 37.90, 32.18, 28.34, 23.85; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{18}H_{18}NO_3$ 296.1281; found 296.1288.



***5,6,10,10-Tetramethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3qa).** The title compound was prepared from 3- 3-(3,4-dimethylphenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 53% yield (41 mg); mp = 225-226 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.19 (s, 1H), 7.62 (s, 1H), 5.52 (s, 1H), 3.09 (s, 2H), 2.57 (s, 2H), 2.46 (s, 3H), 2.42 (s, 3H), 1.20 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.17, 168.34, 152.29, 143.93, 142.83, 137.85, 127.88, 127.33, 125.87, 118.10, 109.31, 74.92, 53.07, 37.74, 32.40, 28.37, 20.99, 19.99; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{20}NO_3$ 310.1438; found 310.1432.

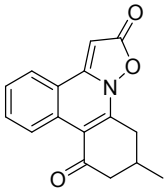


***5,6-Dimethoxy-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3ra).** The title compound was prepared from 3-(3,4-dimethoxyphenyl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 3:1, $R_f$ = 0.5) to afford a yellow solid in 48% yield (41 mg); mp = 170-171 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 10.34 (s, 1H), 8.98 (s, 1H), 8.72 (s, 1H), 4.10 (s, 3H), 4.09 (s, 3H), 3.28 (s, 2H), 2.71 (s, 2H), 1.19 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.12, 157.11, 155.53, 155.52, 151.85, 148.95, 133.25, 122.65, 120.96, 104.32, 103.53, 56.32, 56.20, 54.70, 47.52, 32.94, 28.23, 18.56; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{20}NO_5$ 342.1336; found 342.1340.

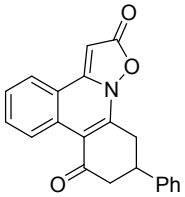


***6,6-dimethyl-6,7-dihydro-2H-benzo[j]isoxazolo[2,3-f]phenanthridine-2,8(5H)-dione*** **(3sa).** The title compound was prepared from 3-(naphthalen-2-yl)isoxazol-5(4*H*)-one and 2-diazo-5,5-dimethylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-

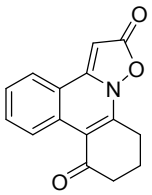
*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a black solid in 63% yield (52 mg); mp = 228-229 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.97 (s, 1H), 8.44 (s, 1H), 8.08 (d, $J$ = 8.5 Hz, 1H), 7.99 (d, $J$ = 8.2 Hz, 1H), 7.67 – 7.58 (m, 2H), 5.81 (s, 1H), 3.12 (s, 2H), 2.63 (s, 2H), 1.24 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.24, 168.04, 152.93, 143.28, 136.29, 131.53, 129.50, 128.72, 128.13, 127.65, 127.11, 126.30, 124.94, 118.09, 108.92, 78.19, 53.01, 37.82, 32.39, 28.39; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{18}NO_3$ 332.1281; found 332.1280.



***10-Methyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3ab).** The title compound was prepared from 3-phenylisoxazol-5(4*H*)-one and 2-diazo-5-methylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 63% yield (42 mg);; mp = 222-223 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.42 (d, $J$ = 8.5 Hz, 1H), 7.90–7.87 (m, 1H), 7.78 (ddd, $J$ = 8.6, 7.2, 1.4 Hz, 1H), 7.60–7.56 (m, 1H), 5.60 (s, 1H), 3.46–3.41 (m, 1H), 2.82–2.75 (m, 2H), 2.50–2.40 (m, 2H), 1.25 (d, $J$ = 6.3 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 196.01, 168.05, 152.21, 144.51, 133.40, 129.78, 128.03, 127.24, 125.80, 119.74, 109.85, 75.94, 47.30, 32.00, 28.12, 21.01; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{14}NO_3$ 268.0968; found 268.0974.

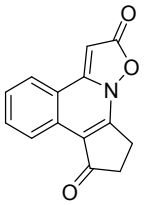


***10-phenyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3ac).** The title compound was prepared from 3-phenylisoxazol-5(4*H*)-one and 2-diazo-5-phenylcyclohexane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 58% yield (48 mg); mp = 191-192 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.46 (d, $J$ = 8.5 Hz, 1H), 7.90 (dd, $J$ = 8.0, 1.2 Hz, 1H), 7.82–7.78 (m, 1H), 7.62–7.58 (m, 1H), 7.43–7.39 (m, 2H), 7.35–7.31 (m, 3H), 5.61 (s, 1H), 3.73–3.58 (m, 2H), 3.31–3.23 (m, 1H), 3.05–2.94 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.18, 167.91, 152.40, 144.29, 141.38, 133.57, 129.82, 129.22, 128.24, 127.76, 127.44, 126.68, 125.90, 119.94, 110.02, 76.25, 46.00, 38.34, 31.70; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{16}NO_3$ 330.1125; found 330.1126.

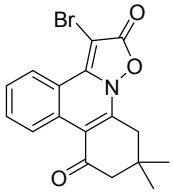


***10,11-Dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(3ad).** The title compound was prepared from 3-phenylisoxazol-5(4*H*)-one and 2-diazocyclohexane-1,3-dione according to the

general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 54% yield (34 mg); mp = 225-226 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.40 (d, $J$ = 8.6 Hz, 1H), 7.87 (dd, $J$ = 8.0, 1.2 Hz, 1H), 7.79–7.74 (m, 1H), 7.60–7.55 (m, 1H), 5.58 (s, 1H), 3.24 (t, $J$ = 6.3 Hz, 2H), 2.75–2.69 (m, 2H), 2.27 (p, $J$ = 6.4 Hz, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.87, 168.11, 152.29, 145.05, 133.45, 129.96, 128.08, 127.49, 125.84, 119.86, 110.31, 76.00, 39.22, 24.43, 20.55; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{12}NO_3$ 254.0812; found 254.0806.

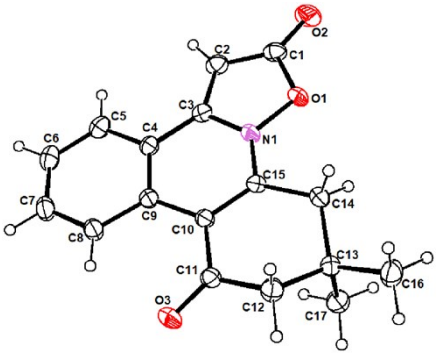


***9,10-Dihydrocyclopenta[c]isoxazolo[3,2-a]isoquinoline-2,8-dione*** **(3ae).** The title compound was prepared from 3-phenylisoxazol-5(4*H*)-one and 2-diazocyclopentane-1,3-dione according to the general procedures (synthesis of isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 4:1, $R_f$ = 0.5) to afford a yellow solid in 46% yield (29 mg); mp = 191-192 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.87 (d, $J$ = 8.2 Hz, 1H), 7.94–7.92 (m, 1H), 7.82–7.78 (m, 1H), 7.64–7.60 (m, 1H), 5.68 (s, 1H), 3.31–3.28 (m, 2H), 2.87–2.85 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 199.62, 168.15, 154.23, 153.53, 133.48, 128.65, 128.37, 126.23, 124.63, 120.46, 114.55, 35.04, 22.04; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}NO_3$ 240.0655; found 240.0653.



***3-Bromo-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(4).** The title compound was prepared from isoxazolo[2,3-*f*]phenanthridines and pyridinium tribromide according to the general procedures (synthesis of 3-bromo-isoxazolo[2,3-*f*]phenanthridines) and purified by column chromatography (petroleum ether/ethyl acetate 8:1, $R_f$ = 0.5) to afford a brown solid in 78% yield (272 mg); mp = 170-171 ºC; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.42 (d, $J$ = 8.6 Hz, 1H), 8.93 (d, $J$ = 8.2 Hz, 1H), 7.81–7.77 (m, 1H), 7.63–7.58 (m, 1H), 3.08 (s, 2H), 2.58 (s, 2H), 1.21 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 195.71, 164.33, 146.09, 143.29, 133.63, 130.20, 127.72, 126.88, 125.61, 120.14, 109.49, 52.87, 37.41, 32.30, 28.32; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{15}BrNO_{33}$ 360.0230; found 360.0233.

## 12. X-ray crystallographic data of compound 3aa




The purified compound **3aa** is dissolved in a mixed solvent of dichloromethane and *n*-hexane, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCDC APEX-2 diffractometer (graphite- monochromated Mo *Kα* radiation, *λ*=0.71073 nm) at 293(2) K.

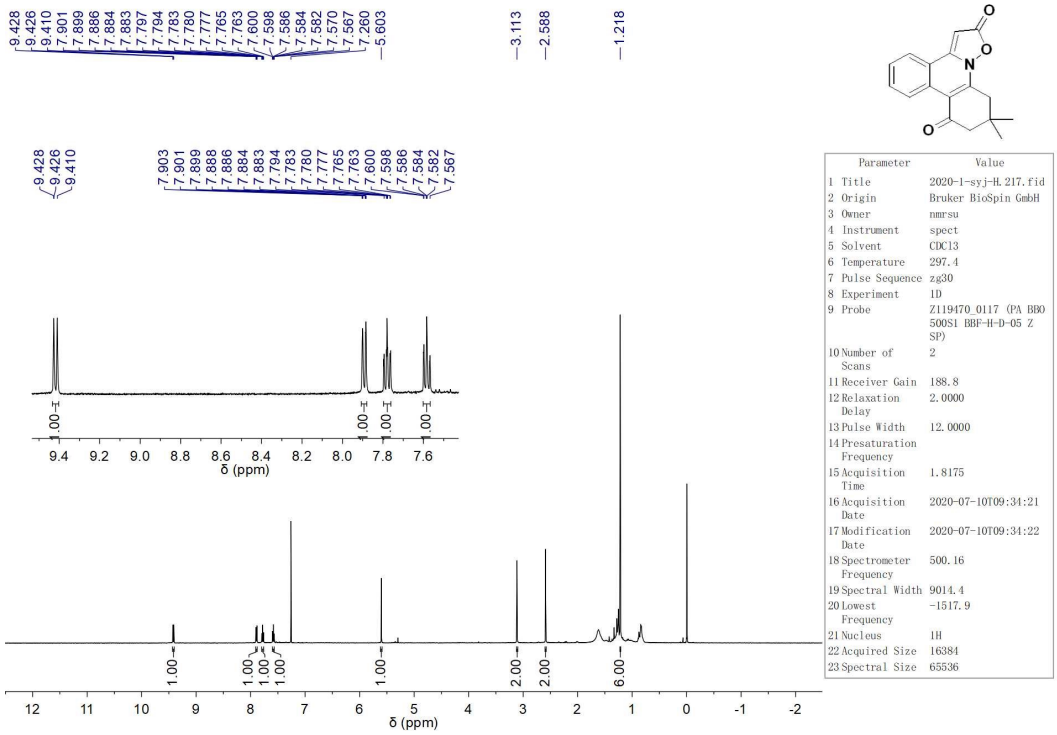
**Figure S1**. ORTEP drawing of compound **3aa** (30% probability for the thermal ellipsoid).

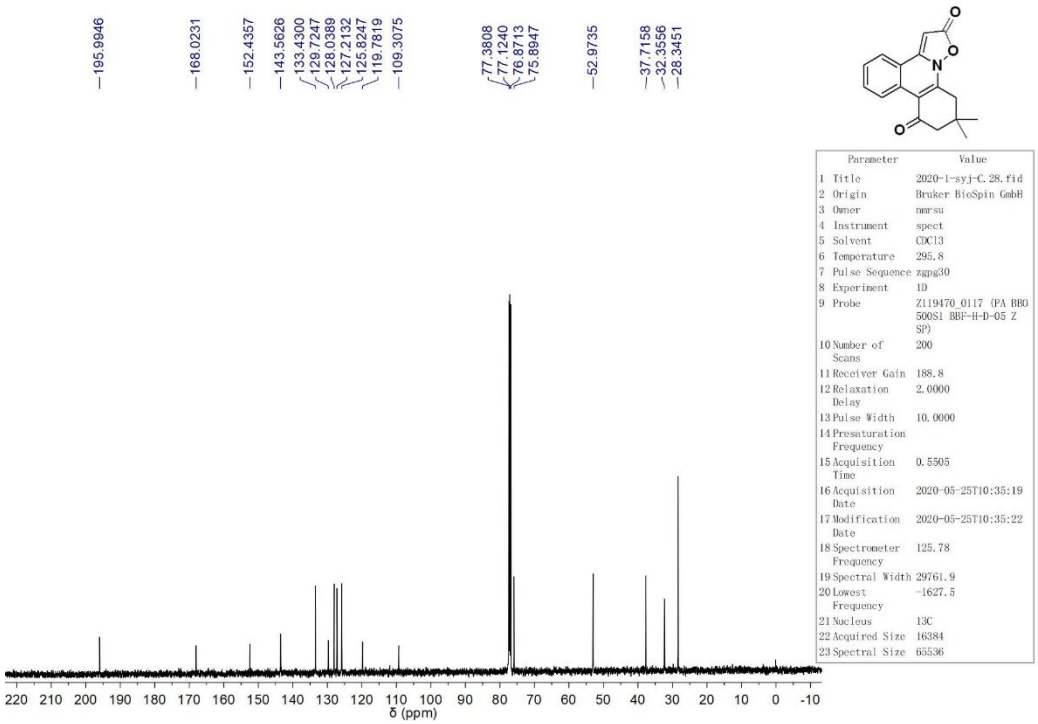
**Table S1**. Crystal data and structure refinement for compound **3aa**.

| | |
|---|---|
| CCDC number | 2045428 |
| Identification code | 20190520a |
| Empirical formula | C17H15NO3 |
| Formula weight | 281.30 |
| Temperature | 293.15 K |
| Wavelength | 0.71073 Å |
| Crystal system | triclinic |
| Space group | P-1 |
| Unit cell dimensions | a = 5.6716(5) Å α= 71.977(4)°.<br>b = 11.2488(11) Å β= 78.405(4)°.<br>c = 11.2777(10) Å γ= 83.699(4)°. |
| Volume | 669.34(11) $Å^3$ |
| Z | 2 |
| Density (calculated) | 1.396 $Mg/m^3$ |
| Absorption coefficient | 0.096 $mm^{-1}$ |
| F(000) | 296.0 |
| Crystal size | 0.23 × 0.21 × 0.2 $mm^3$ |
| Theta range for data collection | 1.908 to 27.926°. |
| Index ranges | $-7 \le h \le 7$, $-14 \le k \le 14$, $-14 \le l \le 14$ |
| Reflections collected | 20030 |
| Independent reflections | 3082 [R(int) = 0.0308] |
| Completeness to theta = 25.242° | 99.5% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3082 / 0 / 192 |
| Goodness-of-fit on $F^2$ | 1.036 |
| Final R indices [I>2sigma(I)] | R1 = 0.0429, wR2 = 0.1052 |
| R indices (all data) | R1 = 0.0588, wR2 = 0.1145 |
| Largest diff. peak and hole | 0.24 and -0.17 $e.Å^{-3}$ |

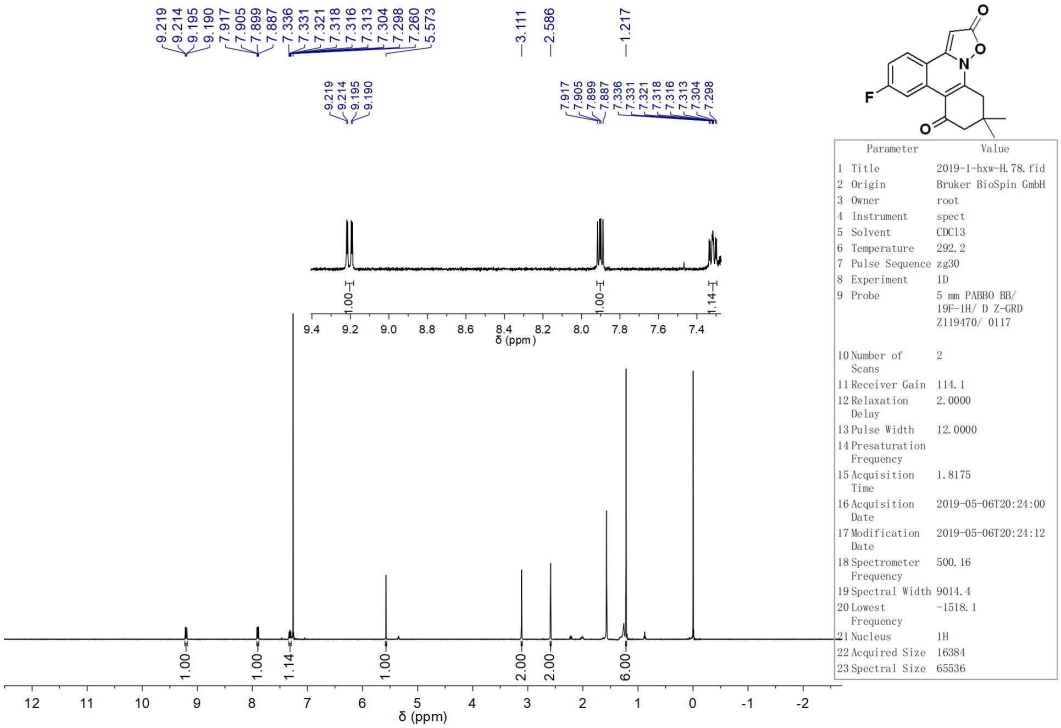
**13. $^{1}H$, $^{13}C$ and/or $^{19}F$ NMR spectra for all compounds**

***10,10-Dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3aa)**



***6-Fluoro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3ba)**




| Parameter | Value |
|---|---|
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| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 292.2 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 114.1 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-05-06T20:24:00 |
| 17 Modification Date | 2019-05-06T20:24:12 |
| 18 Spectrometer Frequency | 500.16 |
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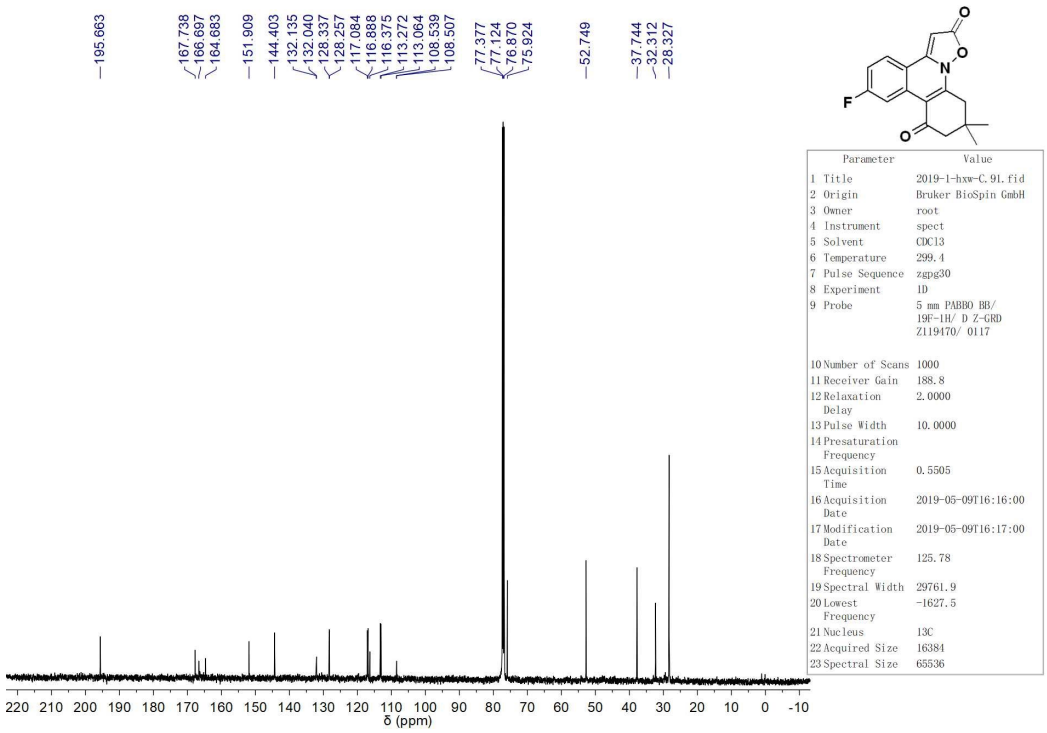
| 20 Lowest Frequency | -1518.1 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

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| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 299.4 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 1000 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
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| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-05-09T16:16:00 |
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| 18 Spectrometer Frequency | 125.78 |
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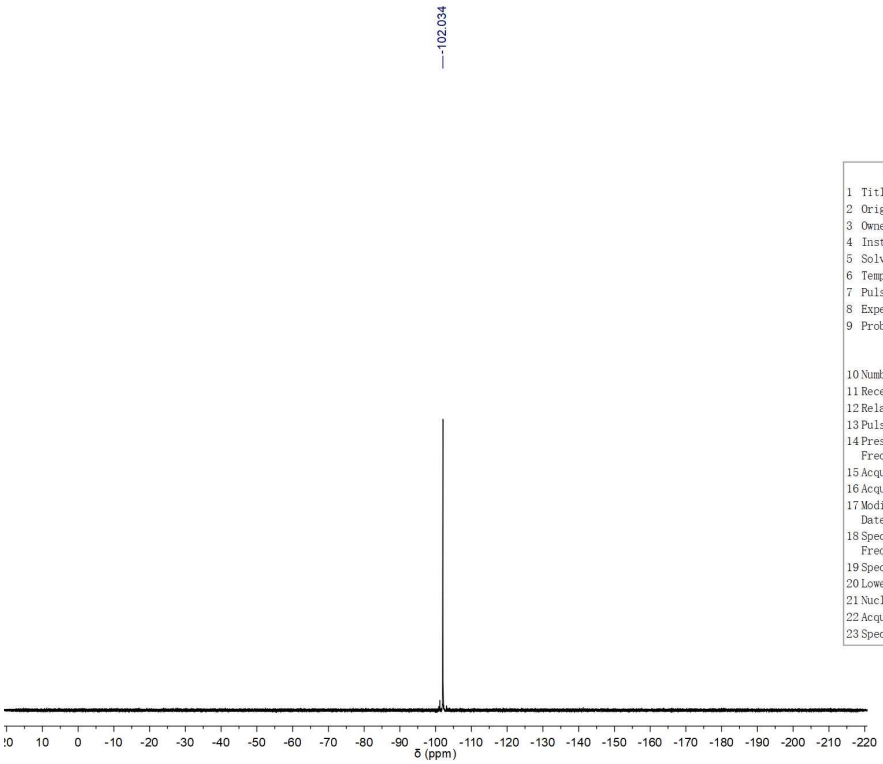
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |




| Parameter | | Value |
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| 3 | Owner | root |
| 4 | Instrument | spect |
| 5 | Solvent | CDCl3 |
| 6 | Temperature | 297.0 |
| 7 | Pulse Sequence | zgflqn |
| 8 | Experiment | 1D |
| 9 | Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 | Number of Scans | 16 |
| 11 | Receiver Gain | 188.8 |
| 12 | Relaxation Delay | 1.0000 |
| 13 | Pulse Width | 15.0000 |
| 14 | Presaturation Frequency | |
| 15 | Acquisition Time | 0.5767 |
| 16 | Acquisition Date | 2019-05-09T17:45:00 |
| 17 | Modification Date | 2019-05-09T17:46:00 |
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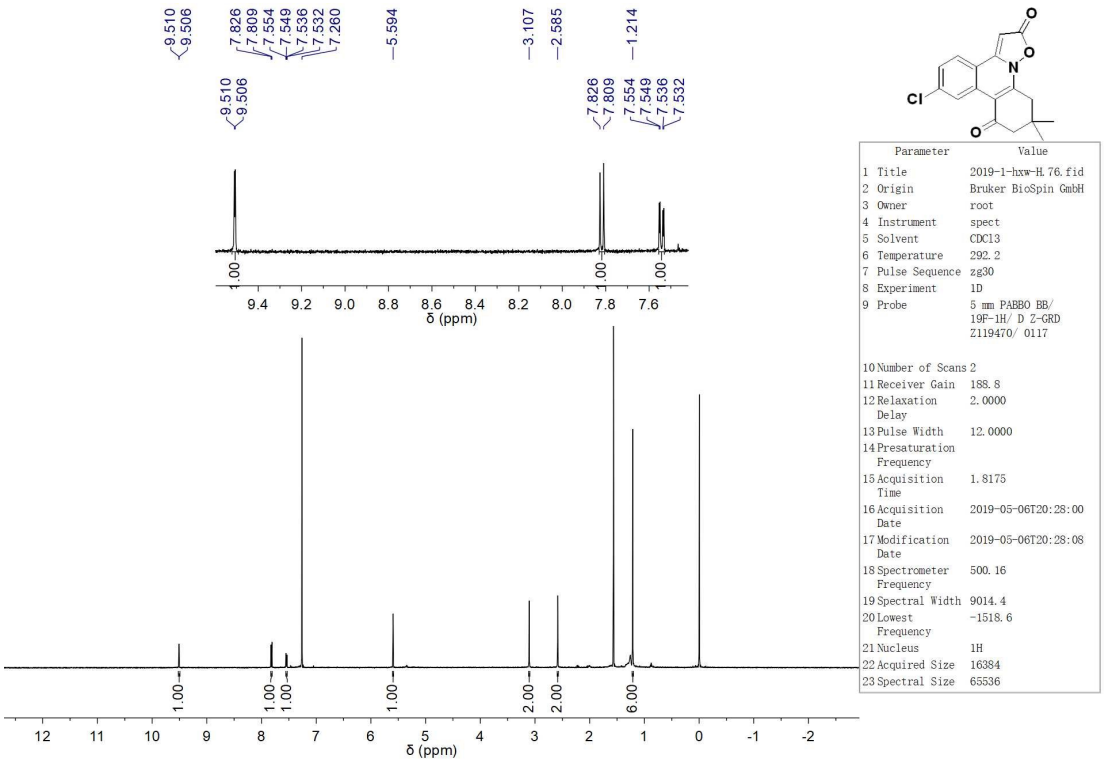
| 20 | Lowest Frequency | -103879.4 |
| 21 | Nucleus | 19F |
| 22 | Acquired Size | 65536 |
| 23 | Spectral Size | 131072 |

***6-Chloro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3ca)**



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| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 292.2 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-05-06T20:28:00 |
| 17 Modification Date | 2019-05-06T20:28:08 |
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| 20 Lowest Frequency | -1518.6 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
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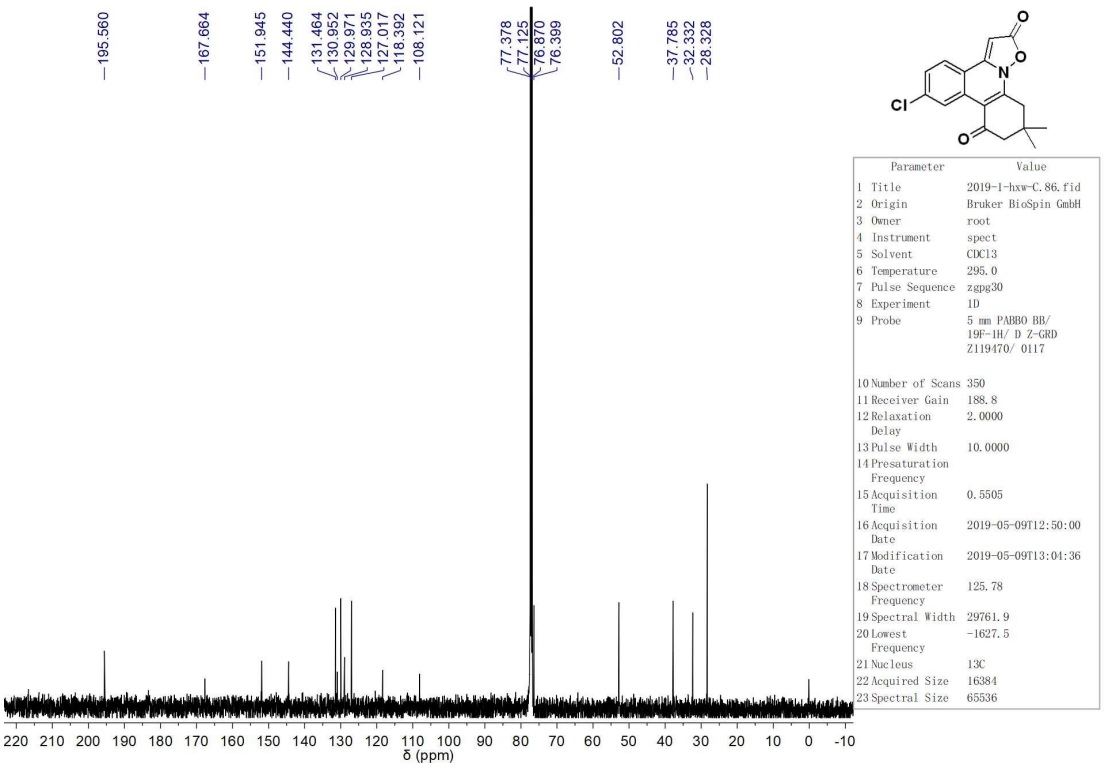




| Parameter | Value |
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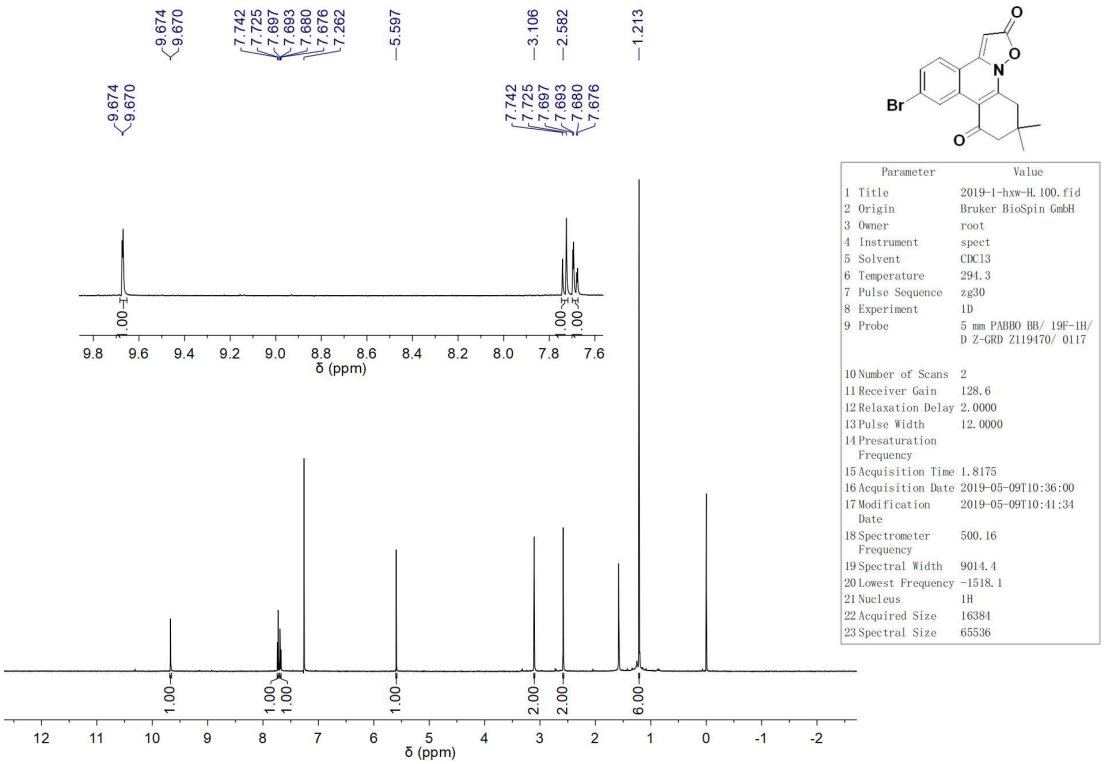
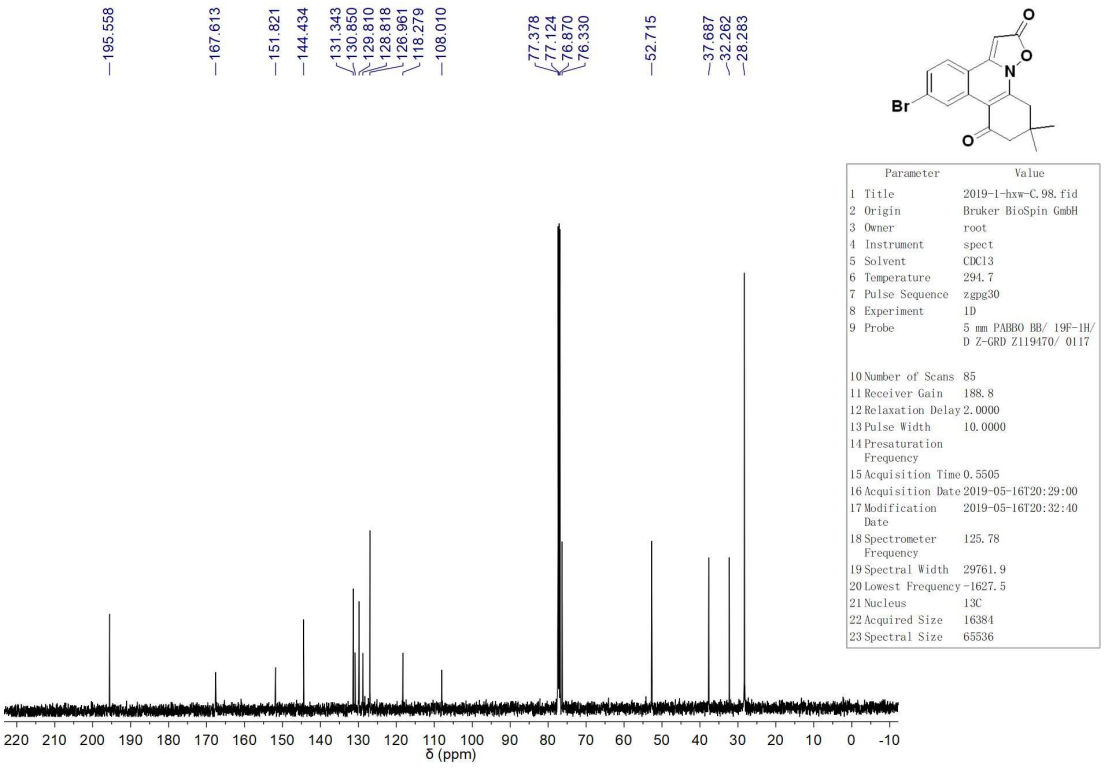
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 295.0 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 350 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-05-09T12:50:00 |
| 17 Modification Date | 2019-05-09T13:04:36 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***6-Bromo-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3da)**

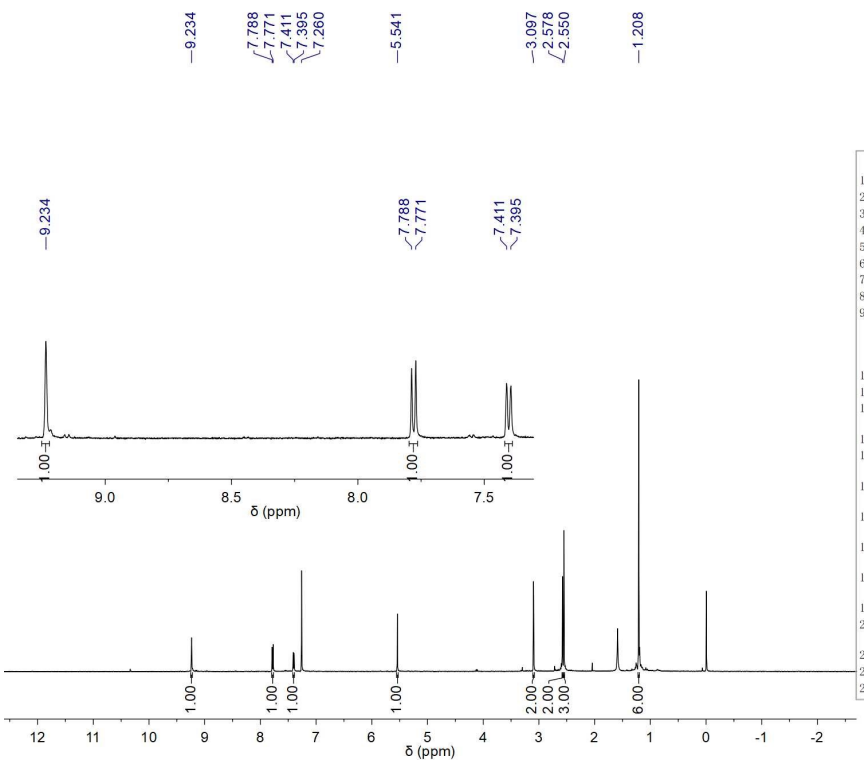



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.100.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.3 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 128.6 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-05-09T10:36:00 |
| 17 Modification Date | 2019-05-09T10:41:34 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.1 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

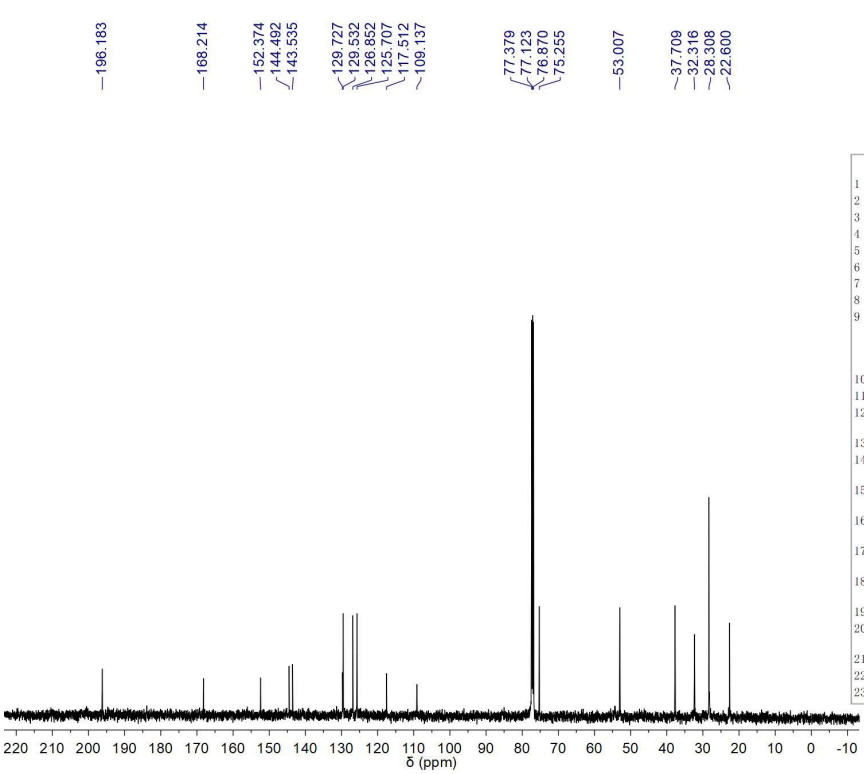



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.98.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.7 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 85 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-05-16T20:29:00 |
| 17 Modification Date | 2019-05-16T20:32:40 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***6,10,10-Trimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3ea)**

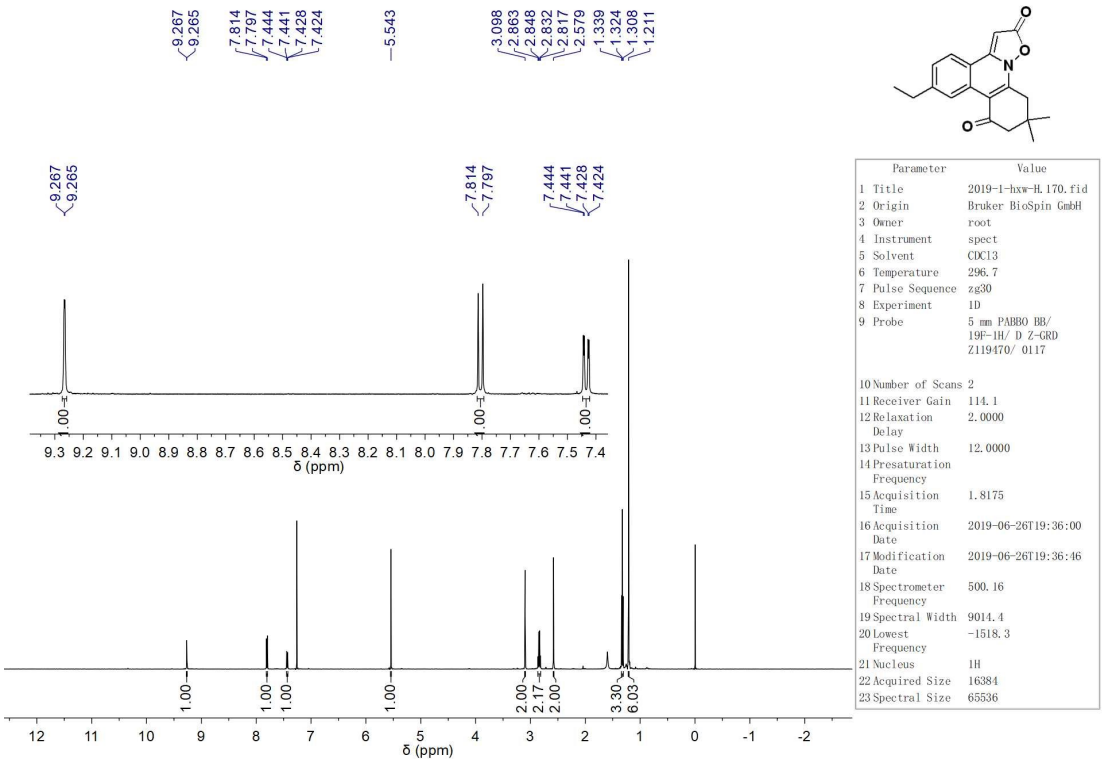


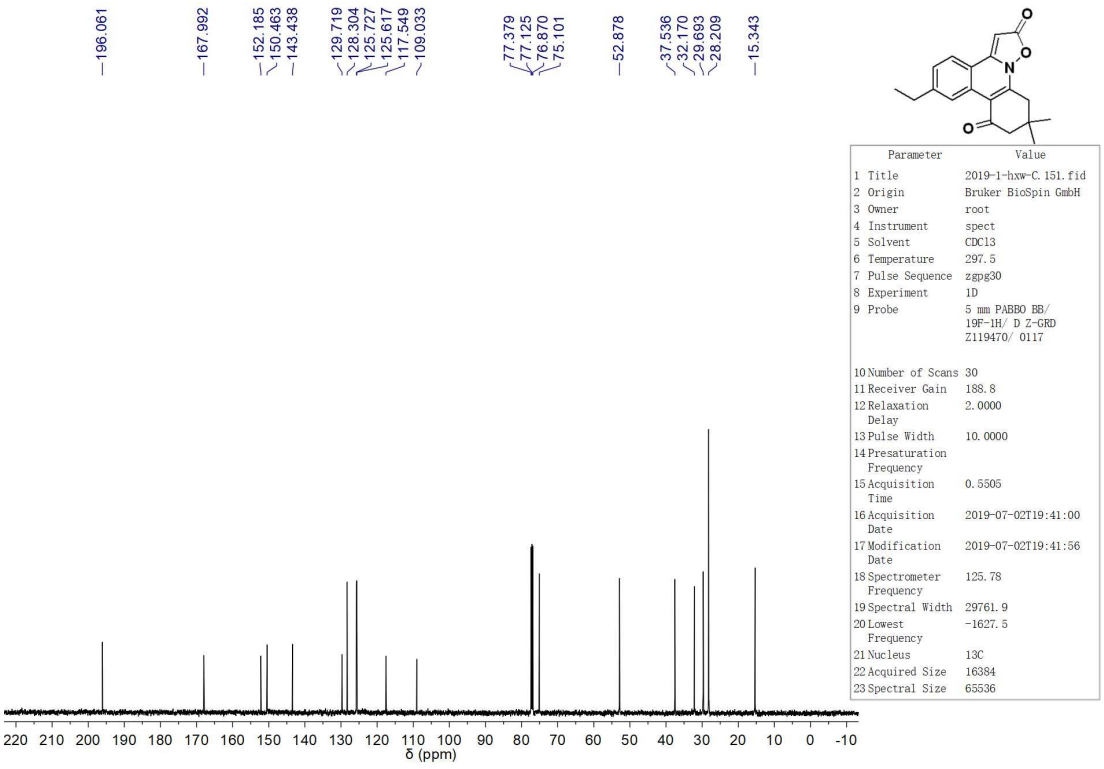

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.94.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.4 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 150.9 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-05-09T10:57:00 |
| 17 Modification Date | 2019-05-09T10:57:46 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1519.1 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



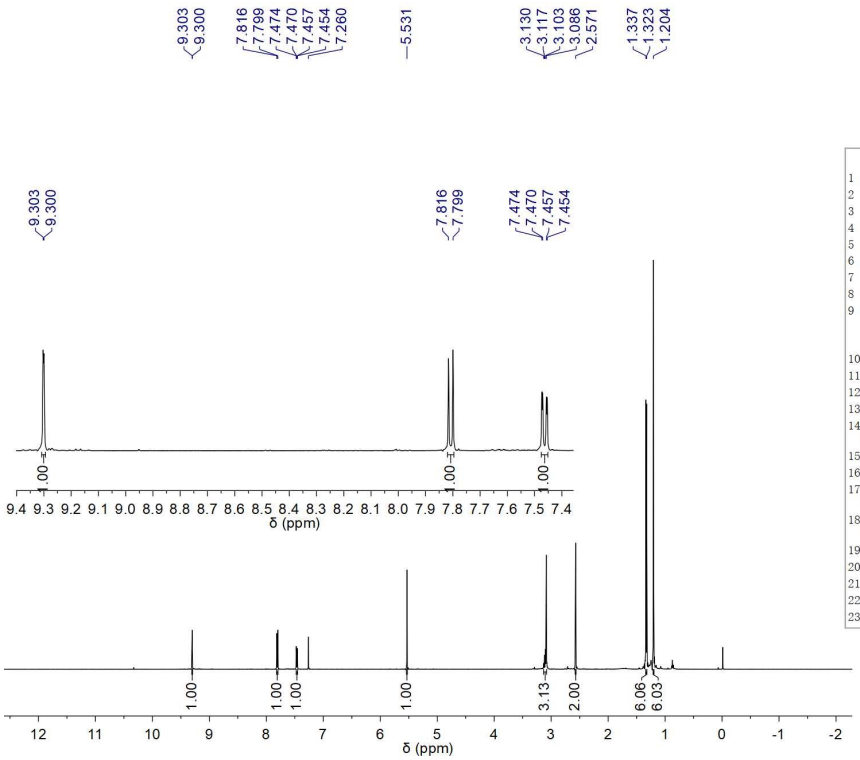

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.99.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.9 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 201 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-05-16T20:43:00 |
| 17 Modification Date | 2019-05-16T20:52:02 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

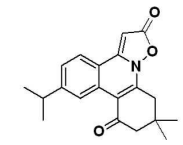
***6-Ethyl-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3fa)**



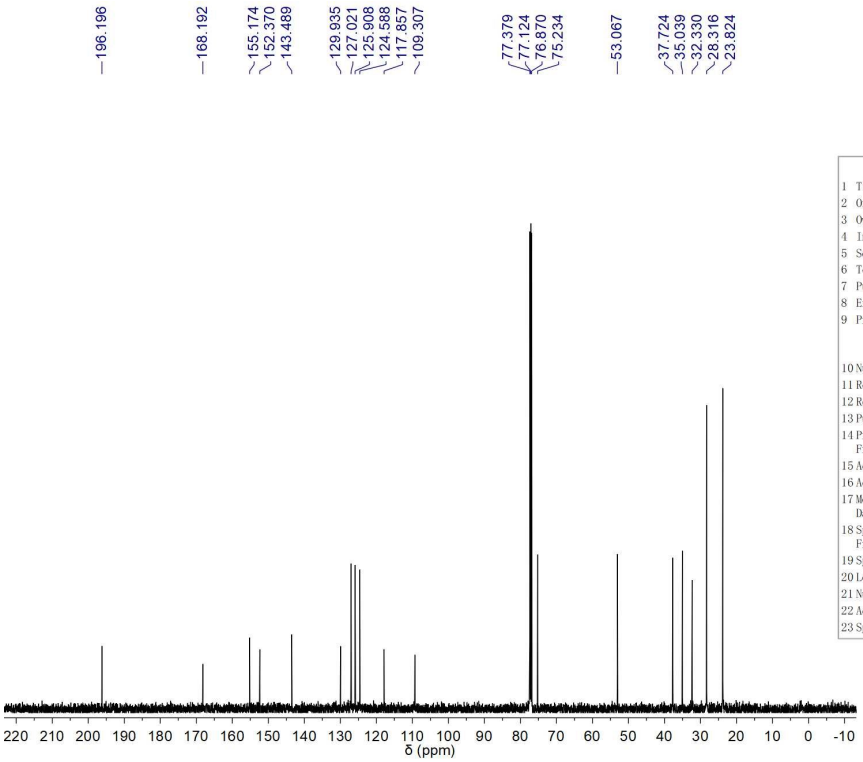



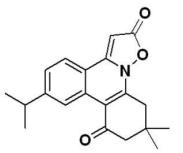
***6-Isopropyl-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3ga)**



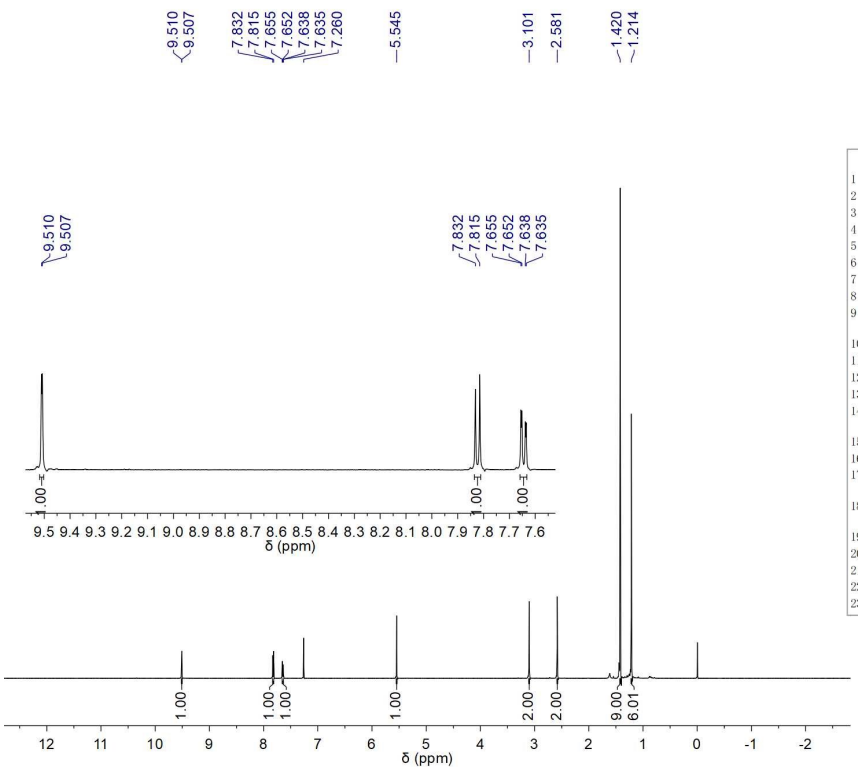
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.336.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 295.9 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 66.5 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-12-10T12:23:00 |
| 17 Modification Date | 2019-12-10T12:23:34 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

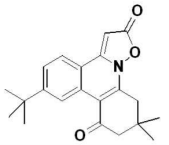


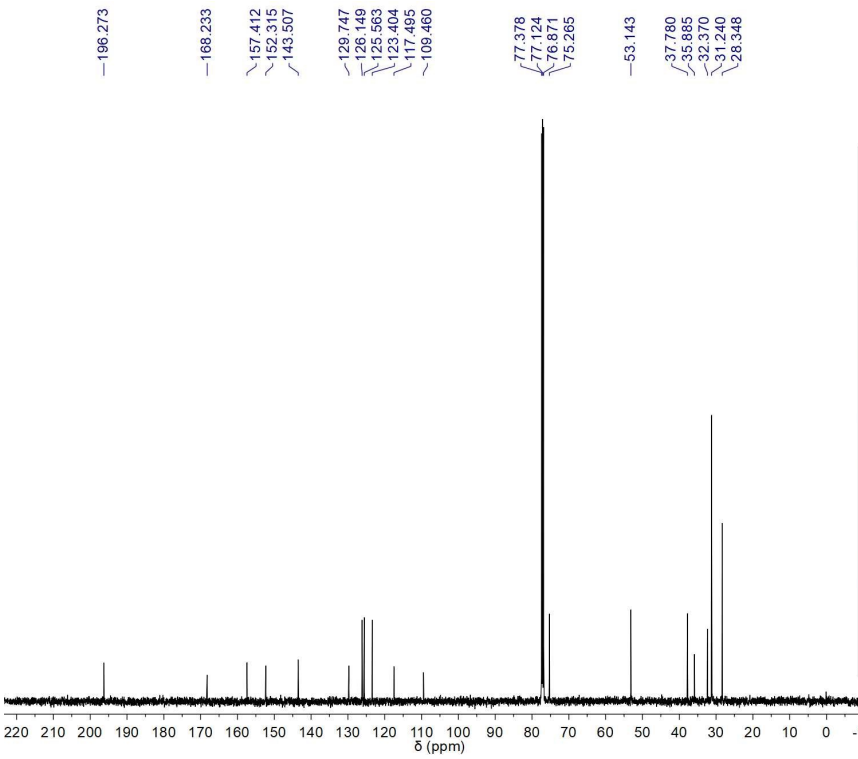
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.263.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 296.3 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 80 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-12-11T11:32:00 |
| 17 Modification Date | 2019-12-11T11:35:20 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

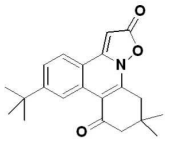
***6-(tert-Butyl)-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3ha)**



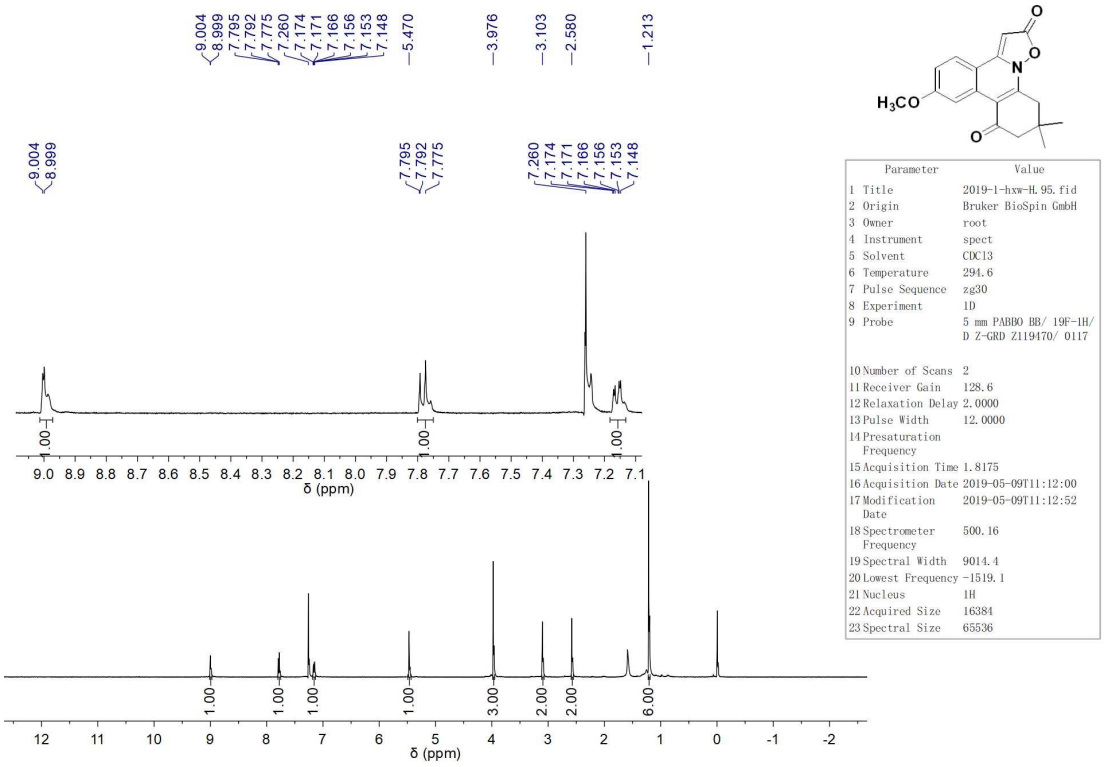
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.283.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.9 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 108.7 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-10-15T10:47:11 |
| 17 Modification Date | 2019-10-15T10:47:12 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



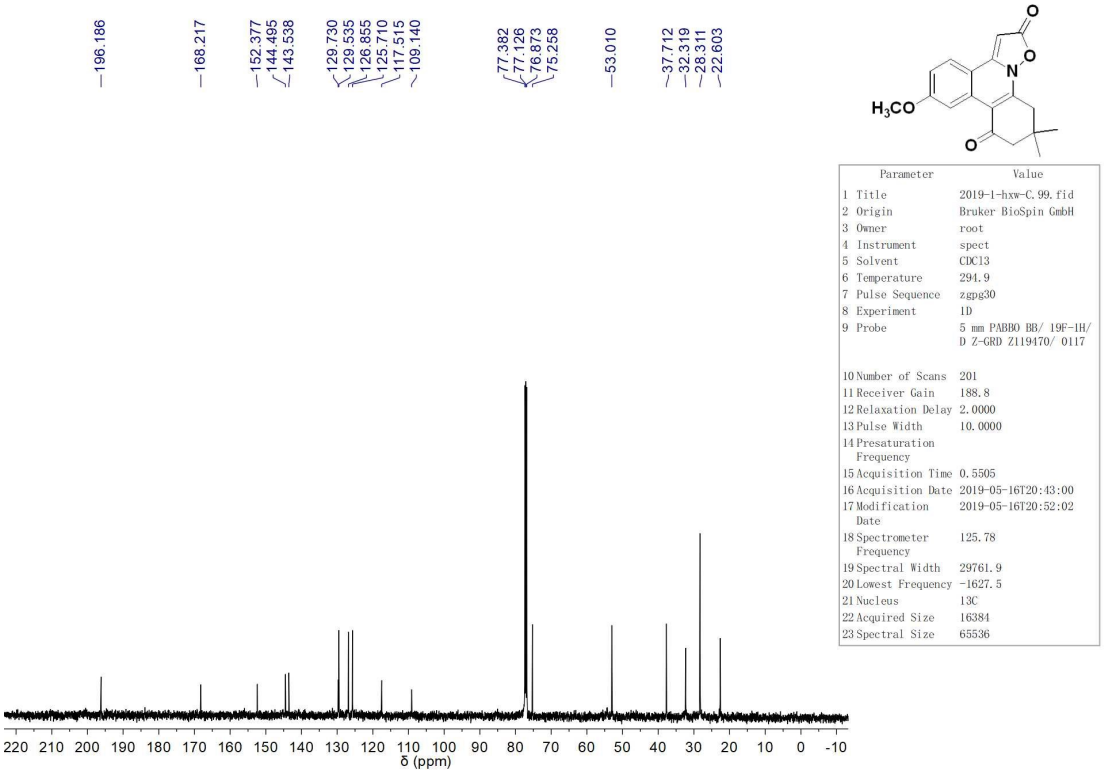



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.233.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 298.4 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 220 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-10-15T10:58:41 |
| 17 Modification Date | 2019-10-15T10:58:44 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***6-Methoxy-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3ia)**

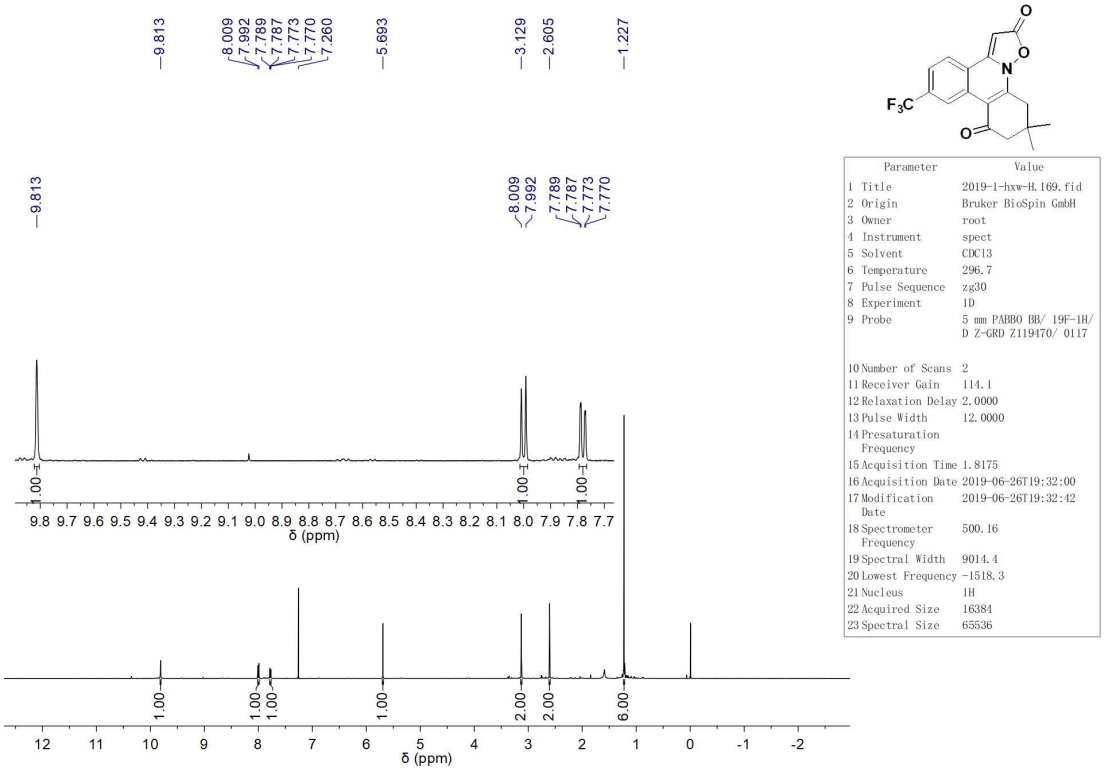



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H. 95. fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.6 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 128.6 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-05-09T11:12:00 |
| 17 Modification Date | 2019-05-09T11:12:52 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1519.1 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



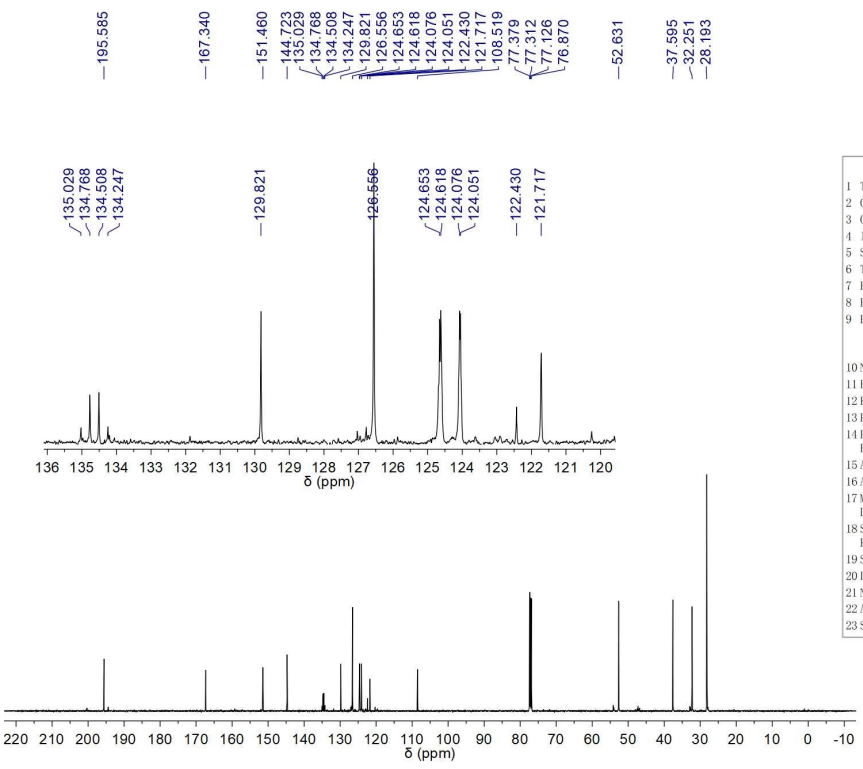

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C. 99. fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.9 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 201 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-05-16T20:43:00 |
| 17 Modification Date | 2019-05-16T20:52:02 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

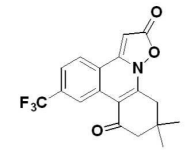
***10,10-Dimethyl-6-(trifluoromethyl)-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3ja)**



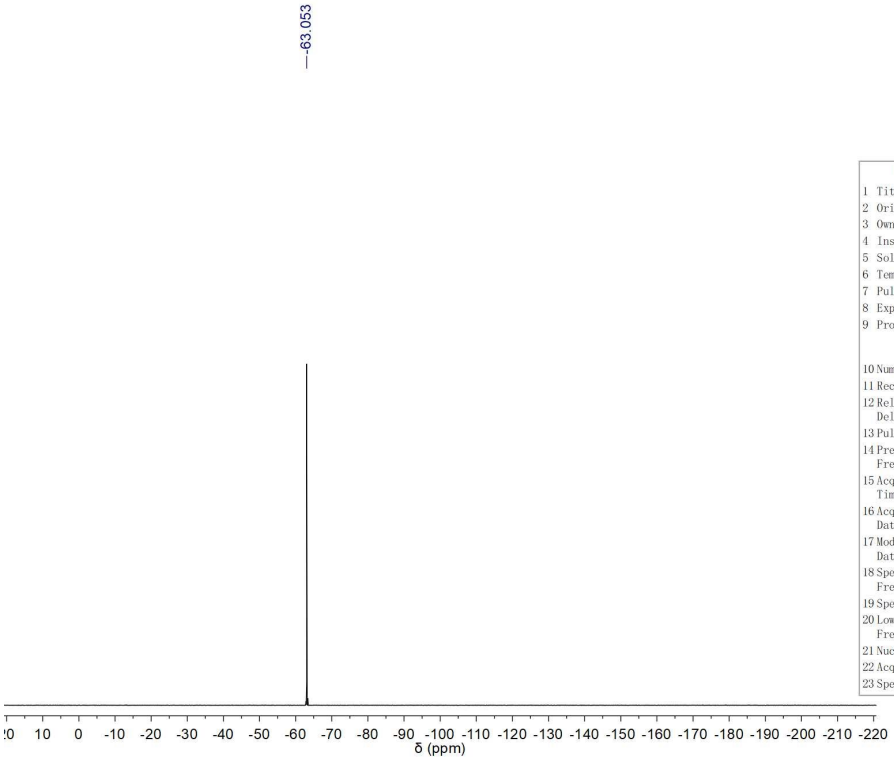



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.169.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 296.7 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 114.1 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-06-26T19:32:00 |
| 17 Modification Date | 2019-06-26T19:32:42 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



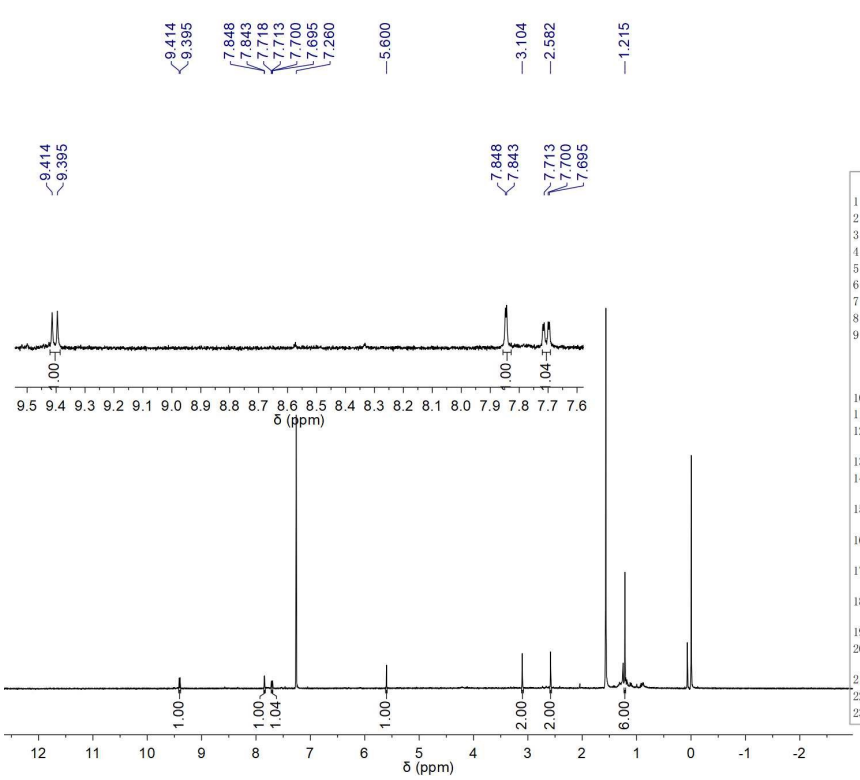



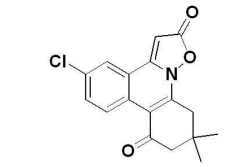
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.152.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.4 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 230 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-07-05T20:37:00 |
| 17 Modification Date | 2019-07-05T20:46:46 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



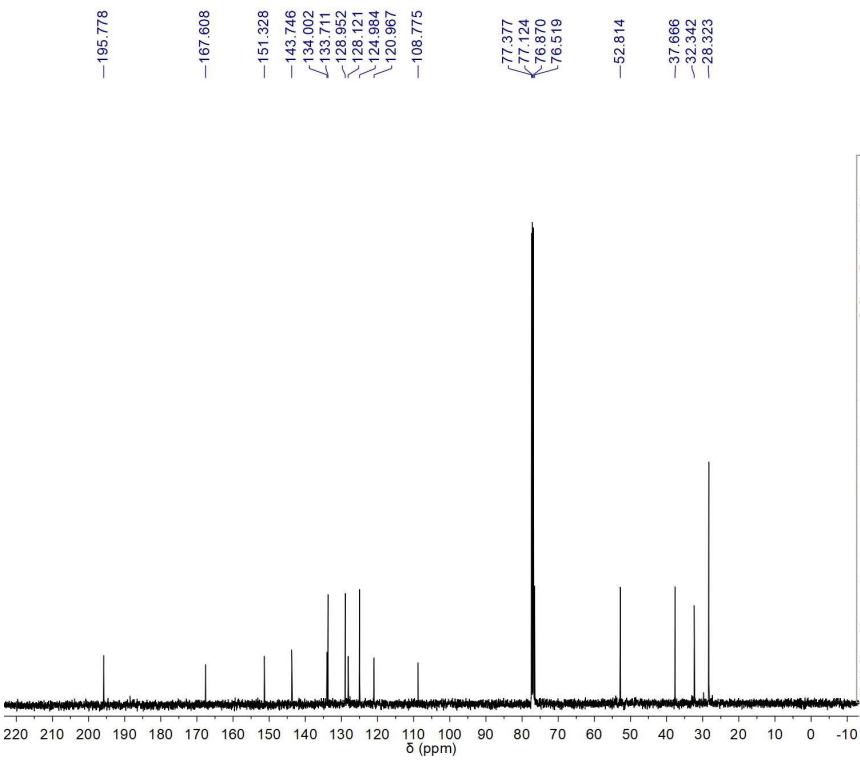

| | Parameter | Value |
|---|---|---|
| 1 | Title | 2020-1-syj-F.18.fid |
| 2 | Origin | Bruker BioSpin GmbH |
| 3 | Owner | nmrsu |
| 4 | Instrument | spect |
| 5 | Solvent | CDCl3 |
| 6 | Temperature | 296.4 |
| 7 | Pulse Sequence | zgflqn |
| 8 | Experiment | 1D |
| 9 | Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 | Number of Scans | 114 |
| 11 | Receiver Gain | 188.8 |
| 12 | Relaxation Delay | 1.0000 |
| 13 | Pulse Width | 15.0000 |
| 14 | Presaturation Frequency | |
| 15 | Acquisition Time | 0.5767 |
| 16 | Acquisition Date | 2020-09-10T11:05:46 |
| 17 | Modification Date | 2020-09-10T11:05:48 |
| 18 | Spectrometer Frequency | 470.57 |
| 19 | Spectral Width | 113636.4 |
| 20 | Lowest Frequency | -103879.4 |
| 21 | Nucleus | 19F |
| 22 | Acquired Size | 65536 |
| 23 | Spectral Size | 131072 |

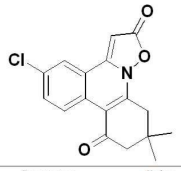
***5-Chloro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3ka)**



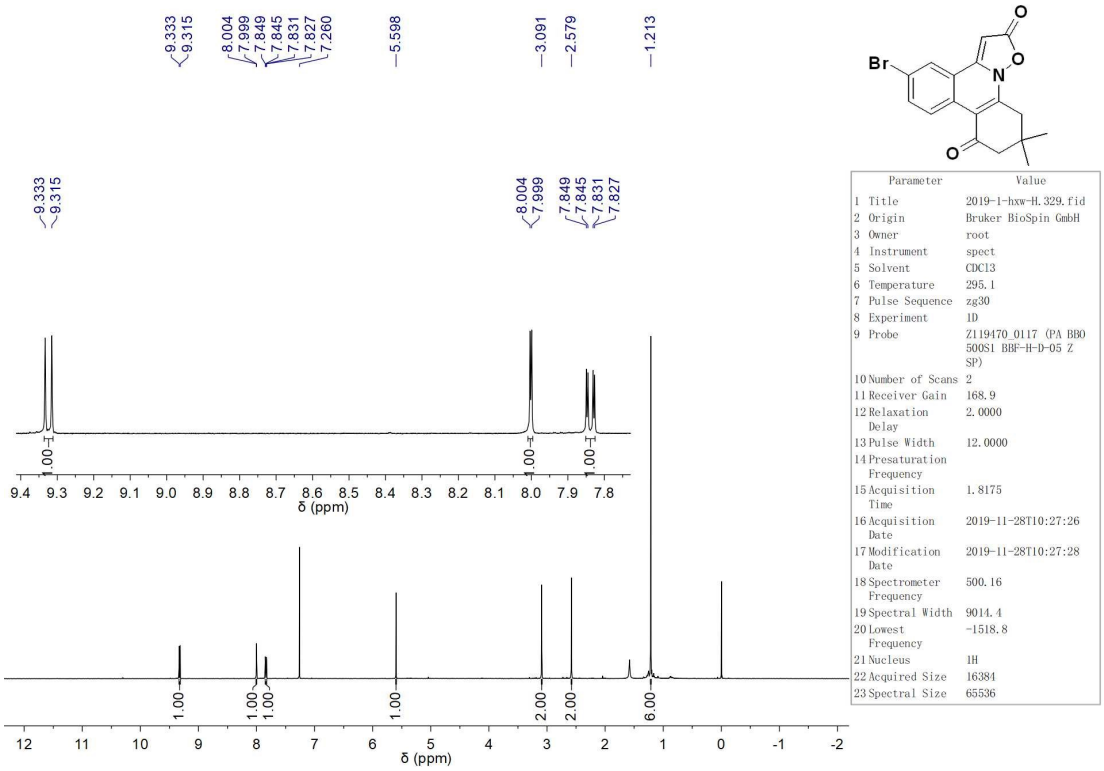
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.148.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.7 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 168.9 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-06-04T11:56:00 |
| 17 Modification Date | 2019-06-04T12:01:58 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.8 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



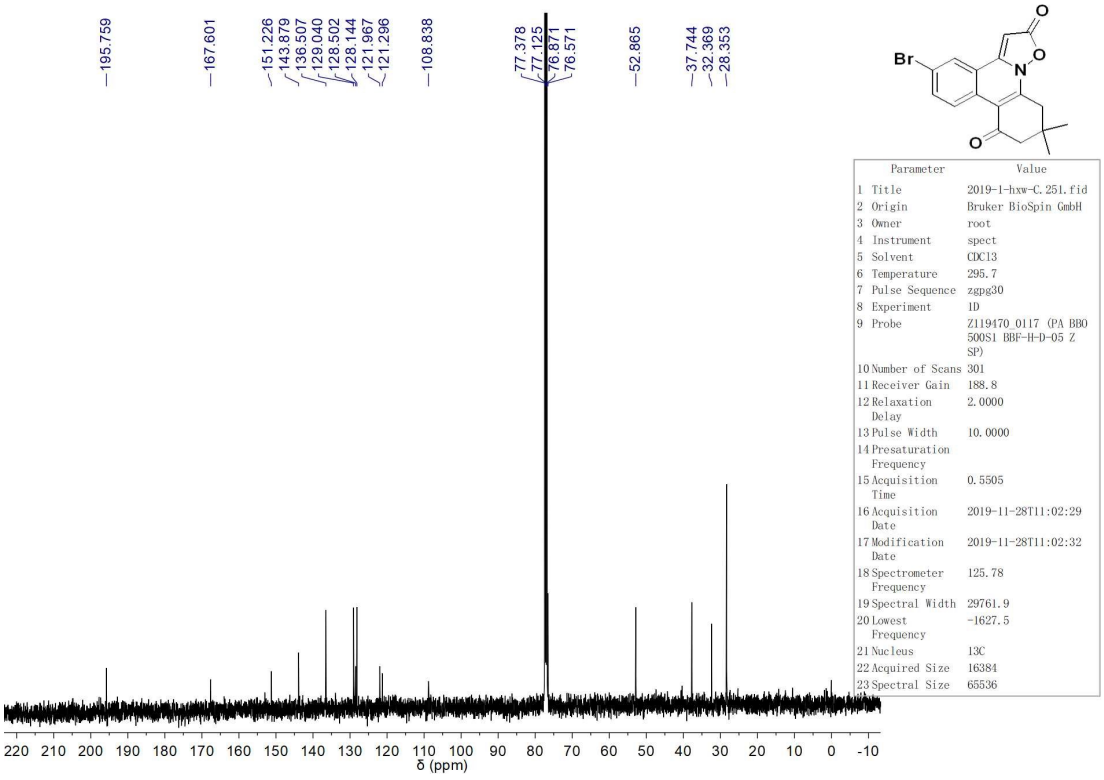



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.153.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.4 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 100 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-07-05T20:49:00 |
| 17 Modification Date | 2019-07-05T20:53:46 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***5-Bromo-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3la)**

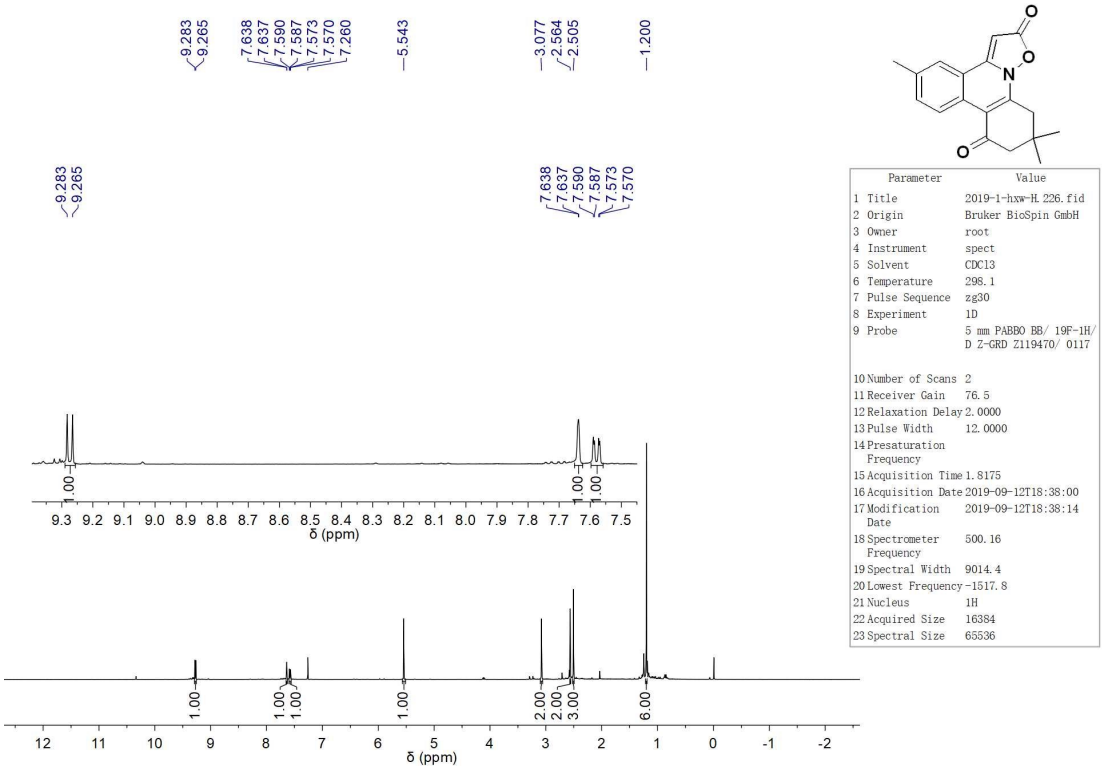



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.329.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 295.1 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 168.9 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-11-28T10:27:26 |
| 17 Modification Date | 2019-11-28T10:27:28 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.8 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

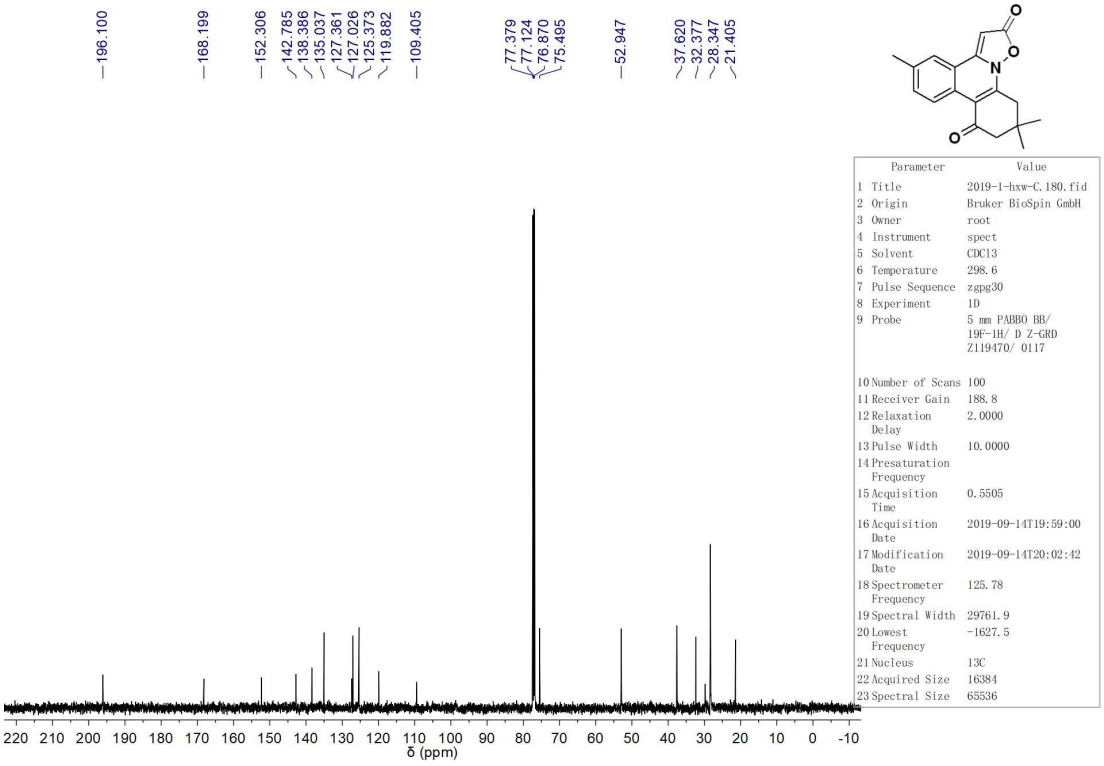



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.251.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 295.7 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 301 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-11-28T11:02:29 |
| 17 Modification Date | 2019-11-28T11:02:32 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***5,10,10-Trimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3ma)**

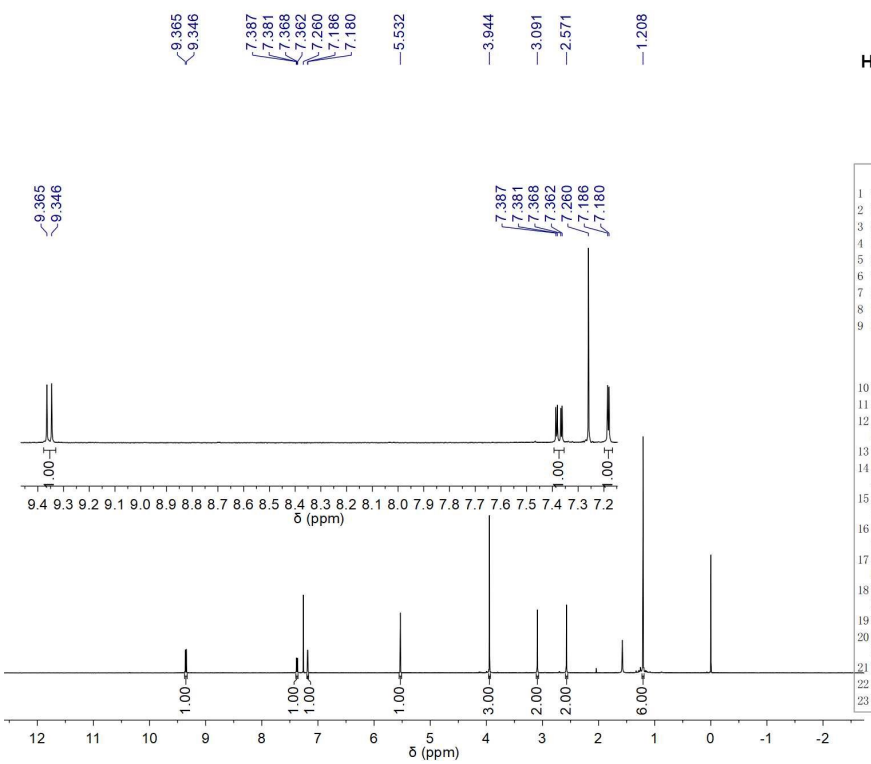


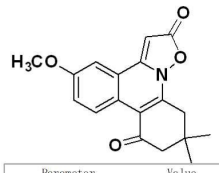

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H 226.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 298.1 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 76.5 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-09-12T18:38:00 |
| 17 Modification Date | 2019-09-12T18:38:14 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1517.8 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



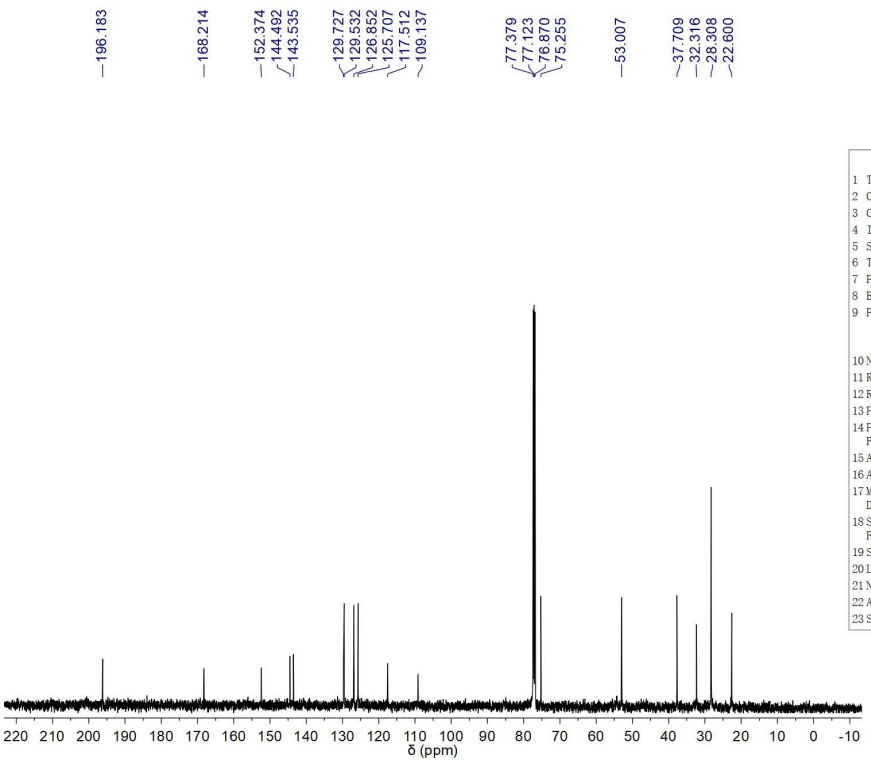

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.180.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 298.6 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 100 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-09-14T19:59:00 |
| 17 Modification Date | 2019-09-14T20:02:42 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

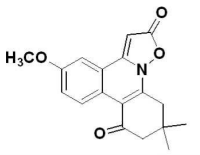
***5-Methoxy-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3na)**



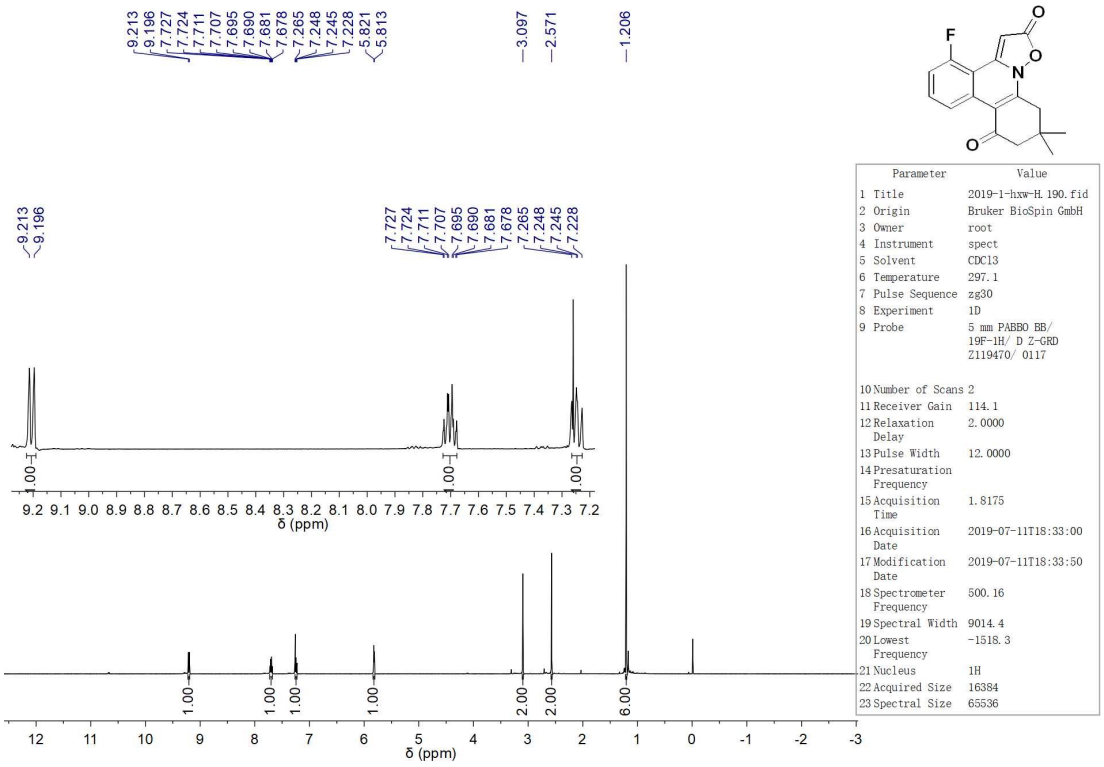
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.200.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 296.8 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 168.9 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-07-22T18:40:00 |
| 17 Modification Date | 2019-07-22T18:40:40 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.8 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



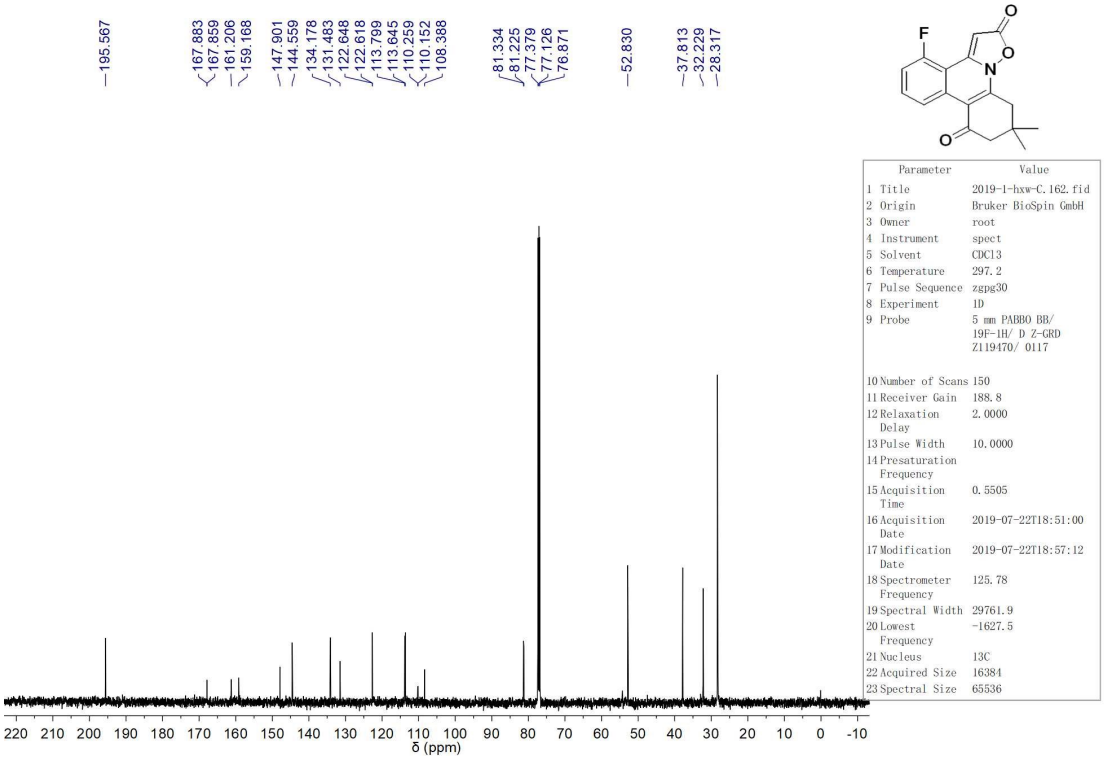



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.99.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 294.9 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 201 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-05-16T20:43:00 |
| 17 Modification Date | 2019-05-16T20:52:02 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

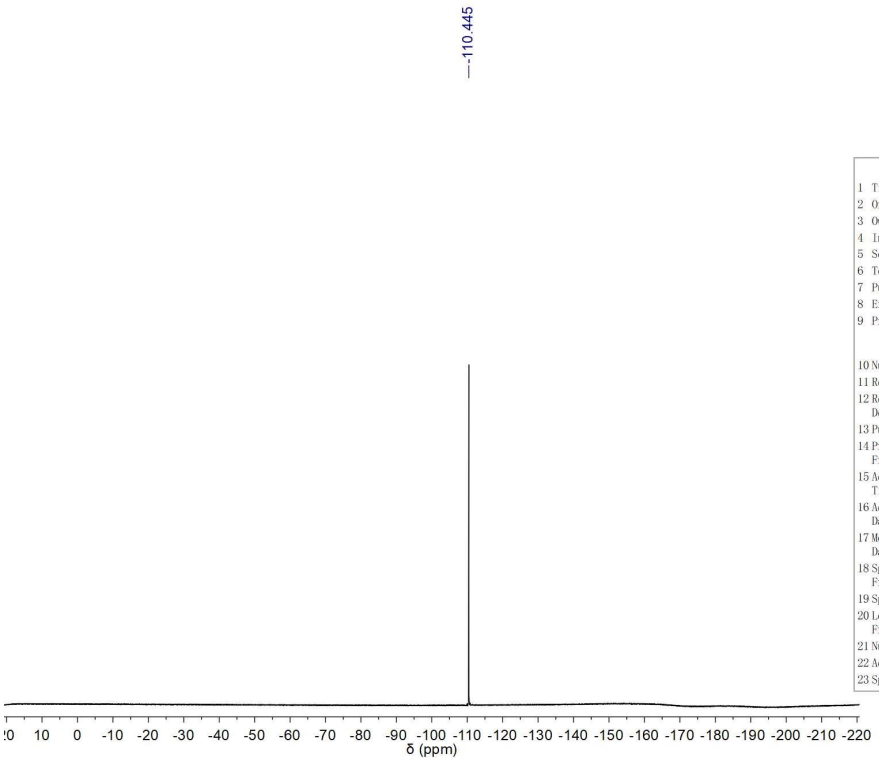
***4-Fluoro-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Table 2, compound 3oa)**




| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H 190.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.1 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 114.1 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-07-11T18:33:00 |
| 17 Modification Date | 2019-07-11T18:33:50 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

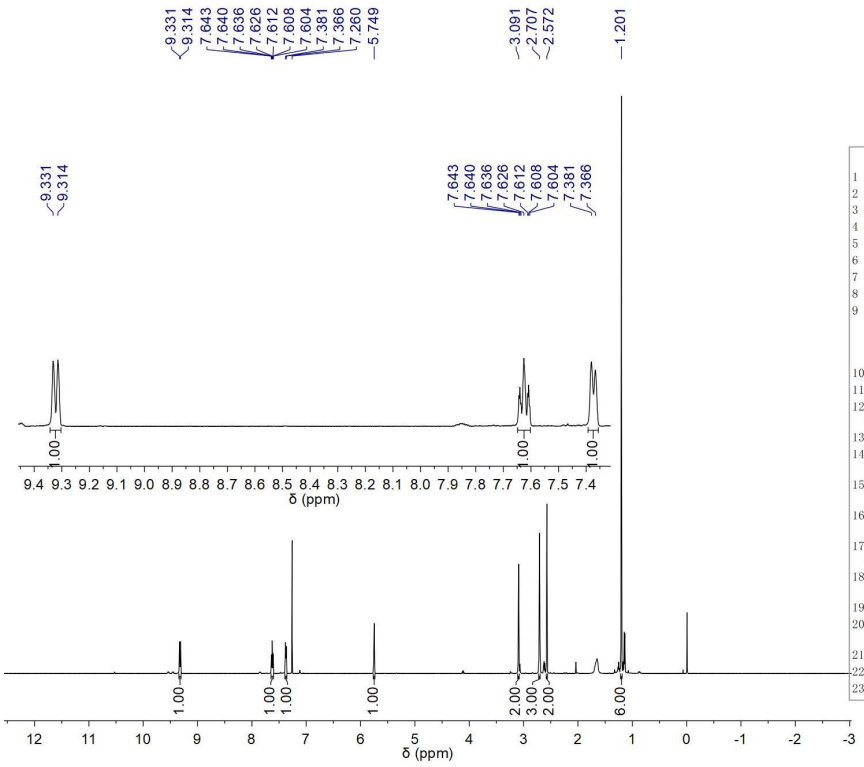


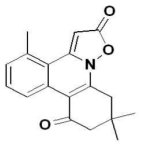

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.162.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.2 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 150 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-07-22T18:51:00 |
| 17 Modification Date | 2019-07-22T18:57:12 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



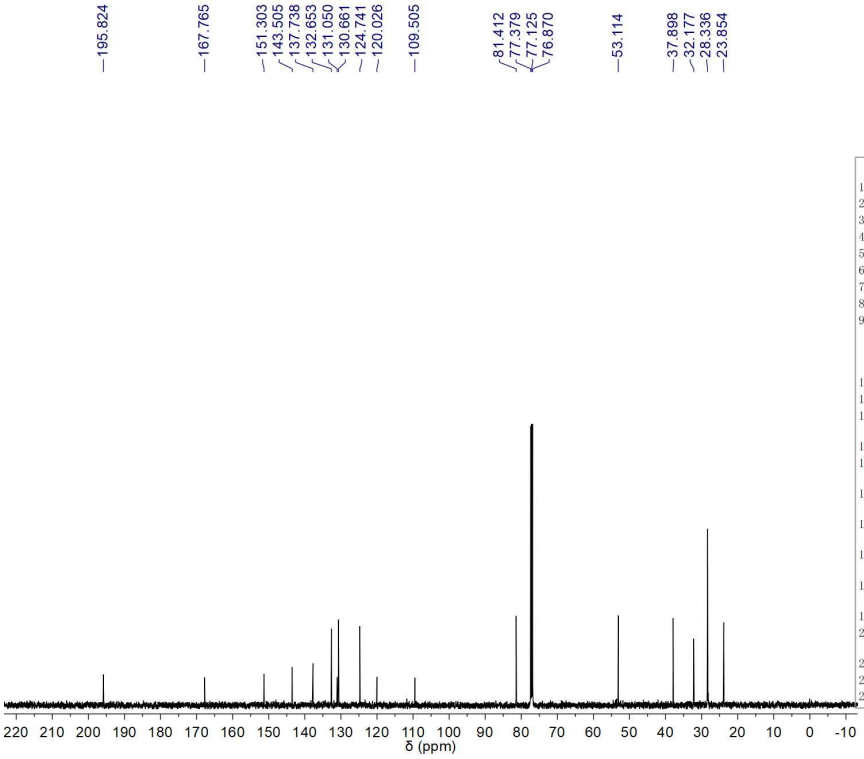

| Parameter | Value |
|---|---|
| 1 Title | 2020-1-syj-F.17.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | nmrsu |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 296.3 |
| 7 Pulse Sequence | zgflqn |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 65 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 1.0000 |
| 13 Pulse Width | 15.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5767 |
| 16 Acquisition Date | 2020-09-10T11:00:29 |
| 17 Modification Date | 2020-09-10T11:00:32 |
| 18 Spectrometer Frequency | 470.57 |
| 19 Spectral Width | 113636.4 |
| 20 Lowest Frequency | -103879.4 |
| 21 Nucleus | 19F |
| 22 Acquired Size | 65536 |
| 23 Spectral Size | 131072 |

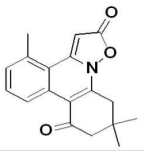
***4,10,10-Trimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3pa)**



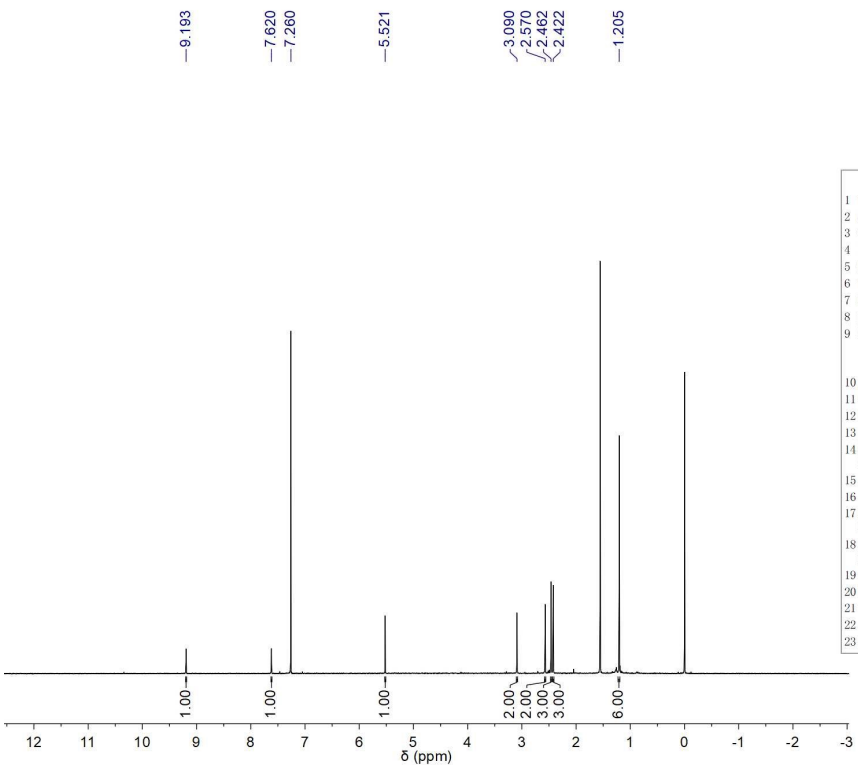
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.107.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.0 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 128.6 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-07-05T20:03:00 |
| 17 Modification Date | 2019-07-05T20:03:14 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.6 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

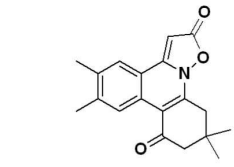


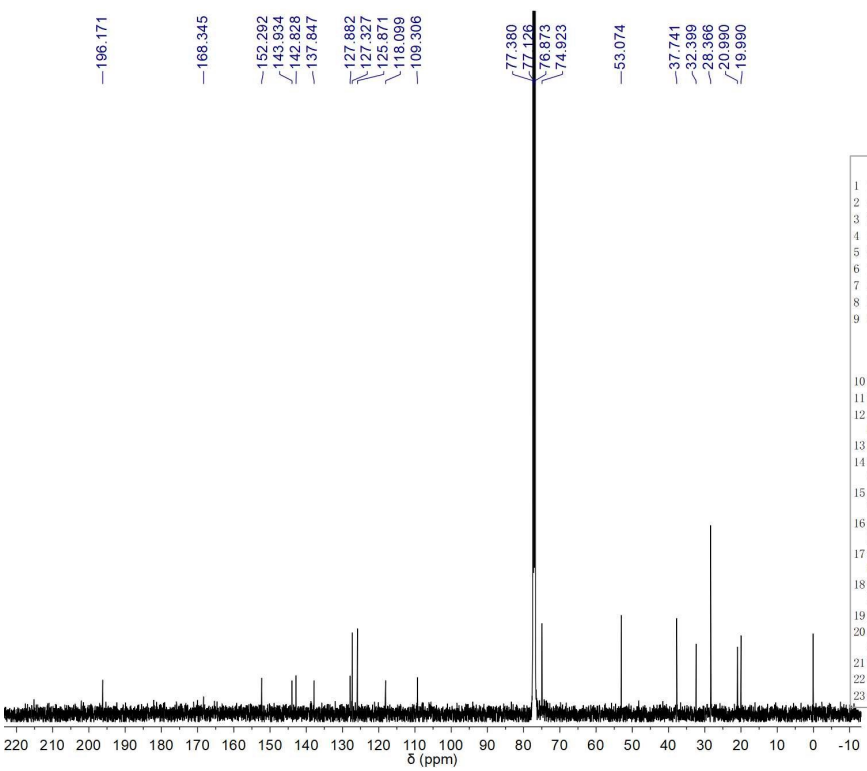
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.161.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.0 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 70 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-07-22T18:44:00 |
| 17 Modification Date | 2019-07-22T18:47:34 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

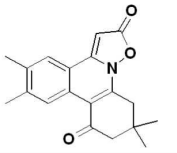
***5,6,10,10-Tetramethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3qa)**



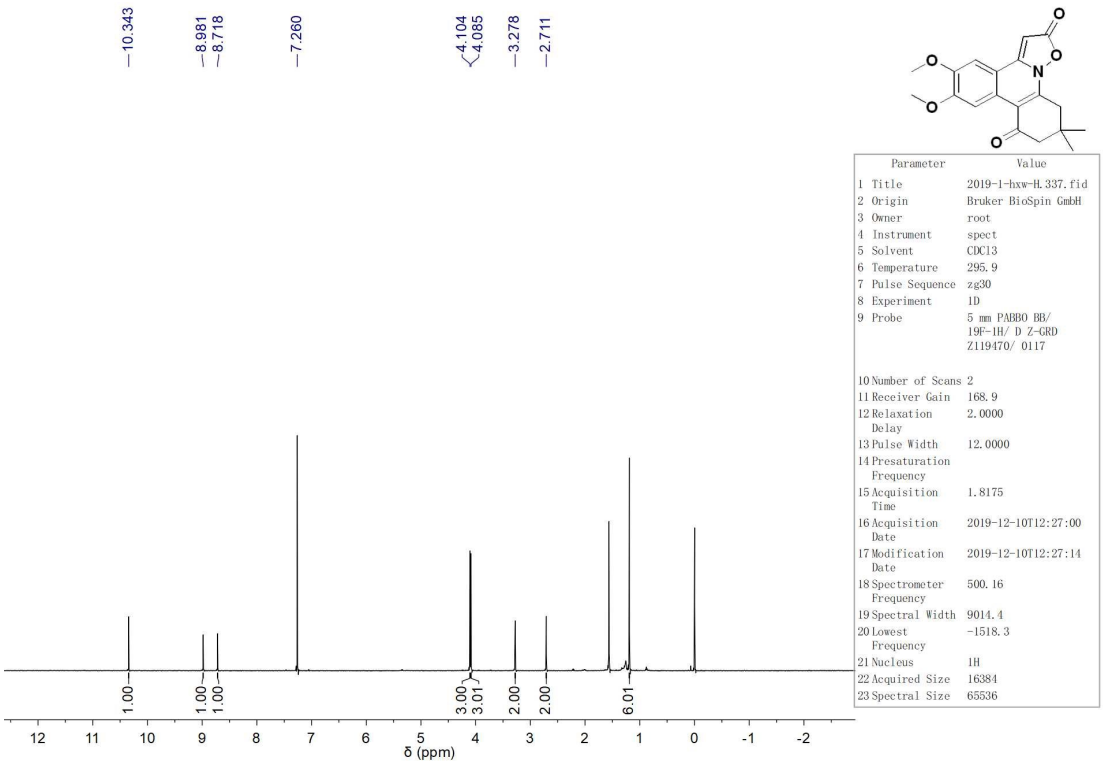
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.262.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.9 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-09-28T23:28:00 |
| 17 Modification Date | 2019-09-28T23:39:34 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



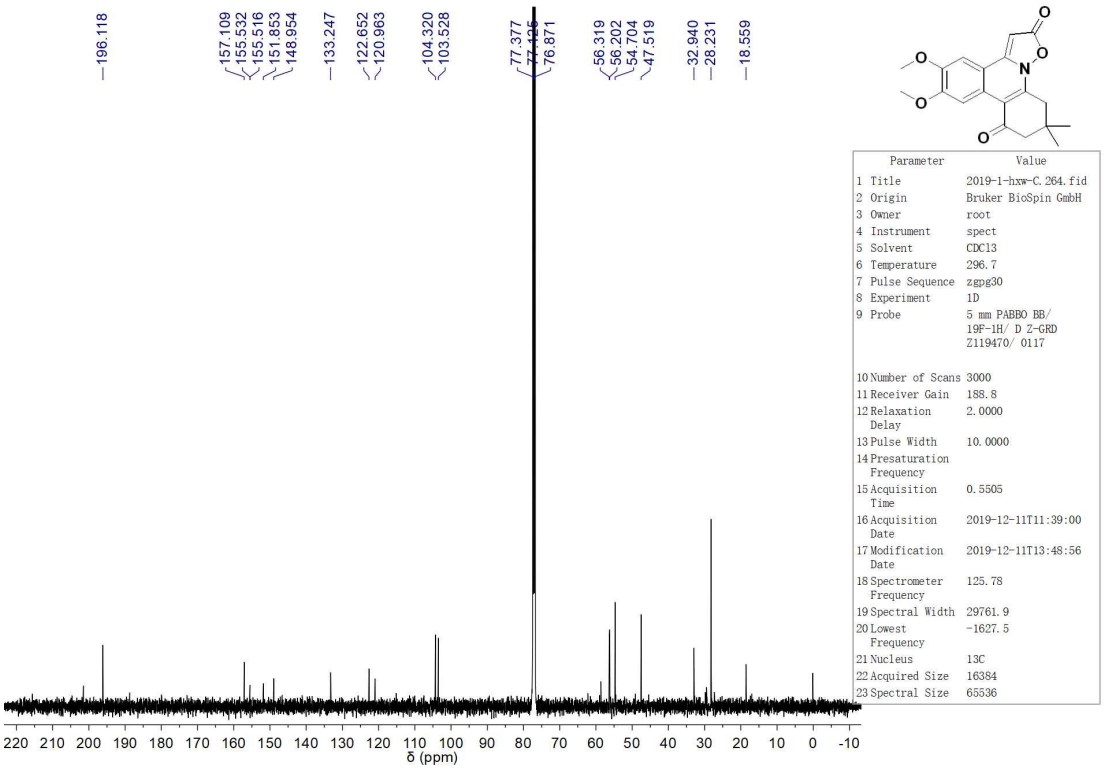



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.219.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 300.0 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 5000 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-09-29T14:28:00 |
| 17 Modification Date | 2019-09-29T14:31:20 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***5,6-Dimethoxy-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (Table 2, compound 3ra)**

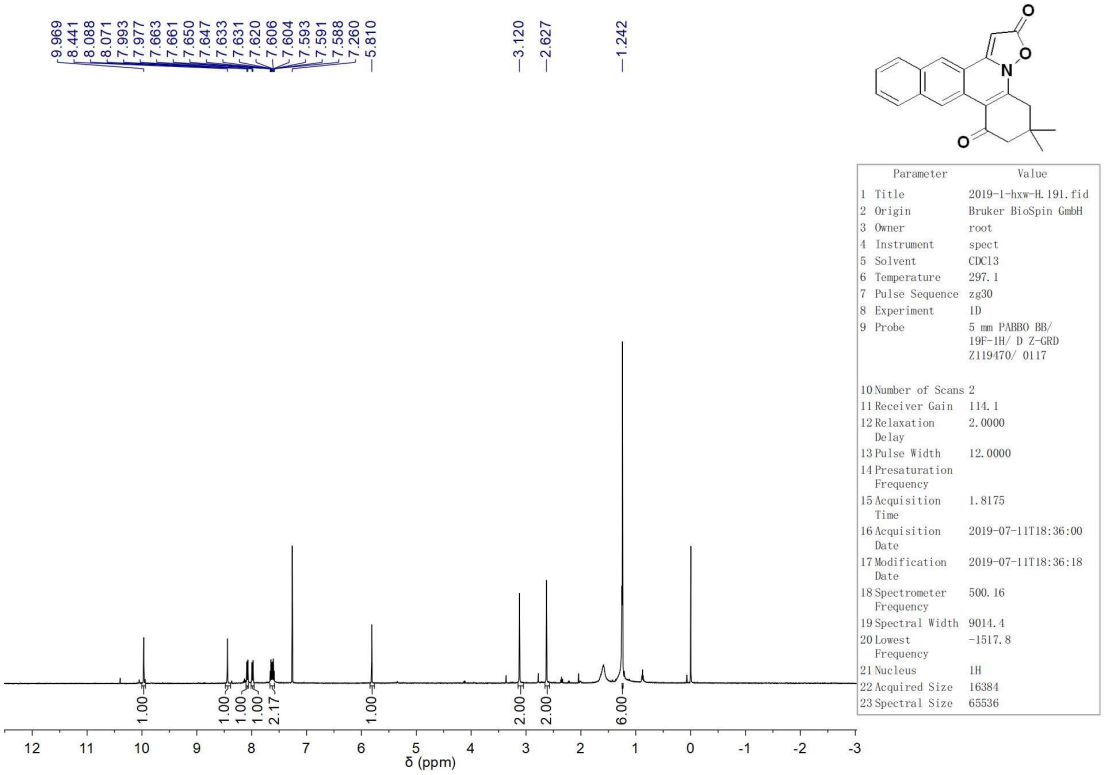



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.337.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 295.9 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 168.9 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-12-10T12:27:00 |
| 17 Modification Date | 2019-12-10T12:27:14 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

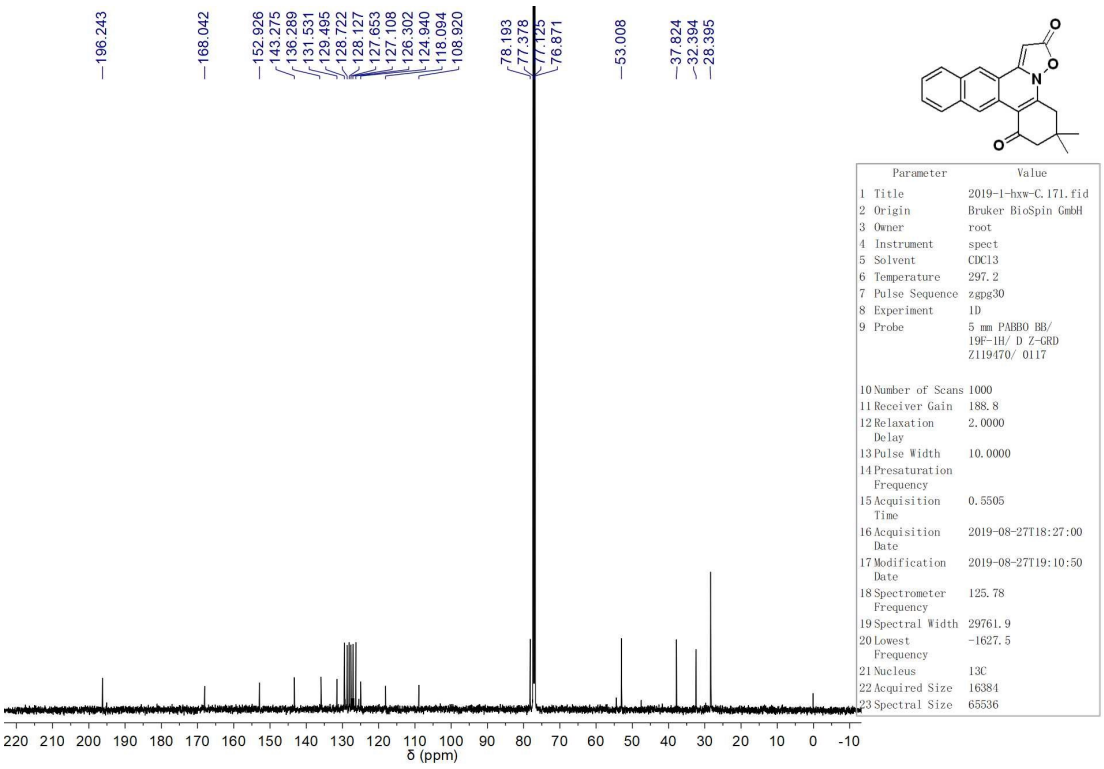



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.264.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 296.7 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 3000 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-12-11T11:39:00 |
| 17 Modification Date | 2019-12-11T13:48:56 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***6,6-Dimethyl-6,7-dihydro-2H-benzo[j]isoxazolo[2,3-f]phenanthridine-2,8(5H)-dione*** **(Table 2, compound 3sa)**

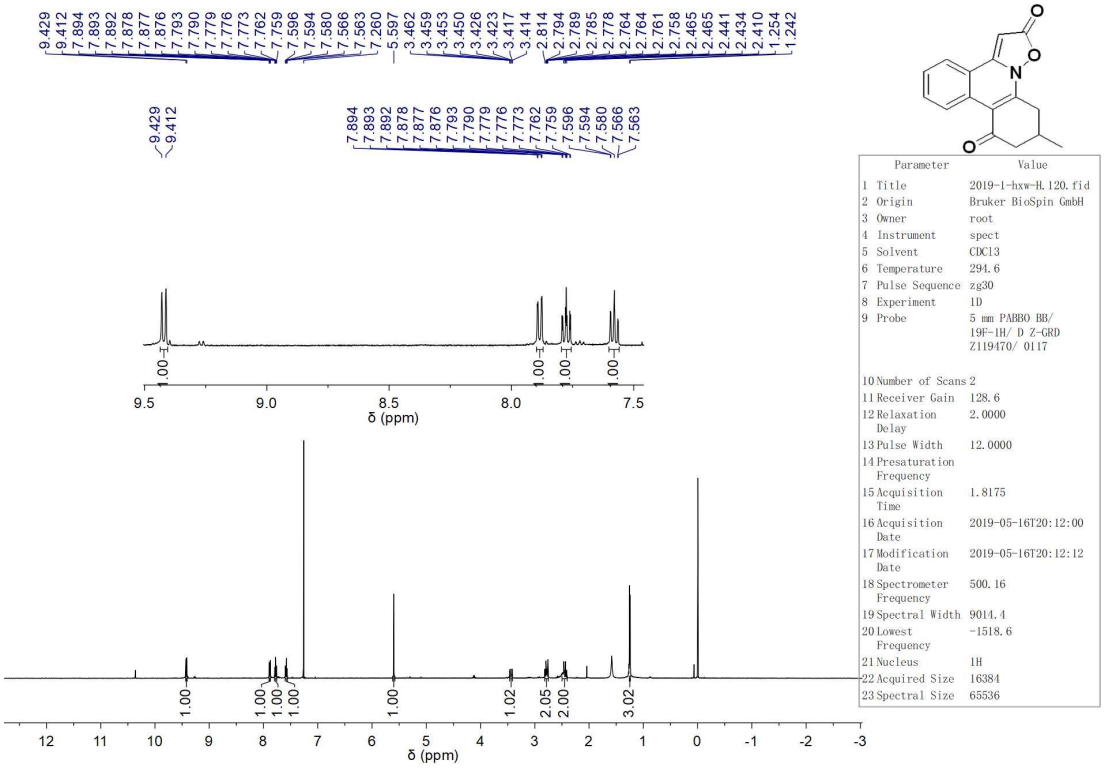


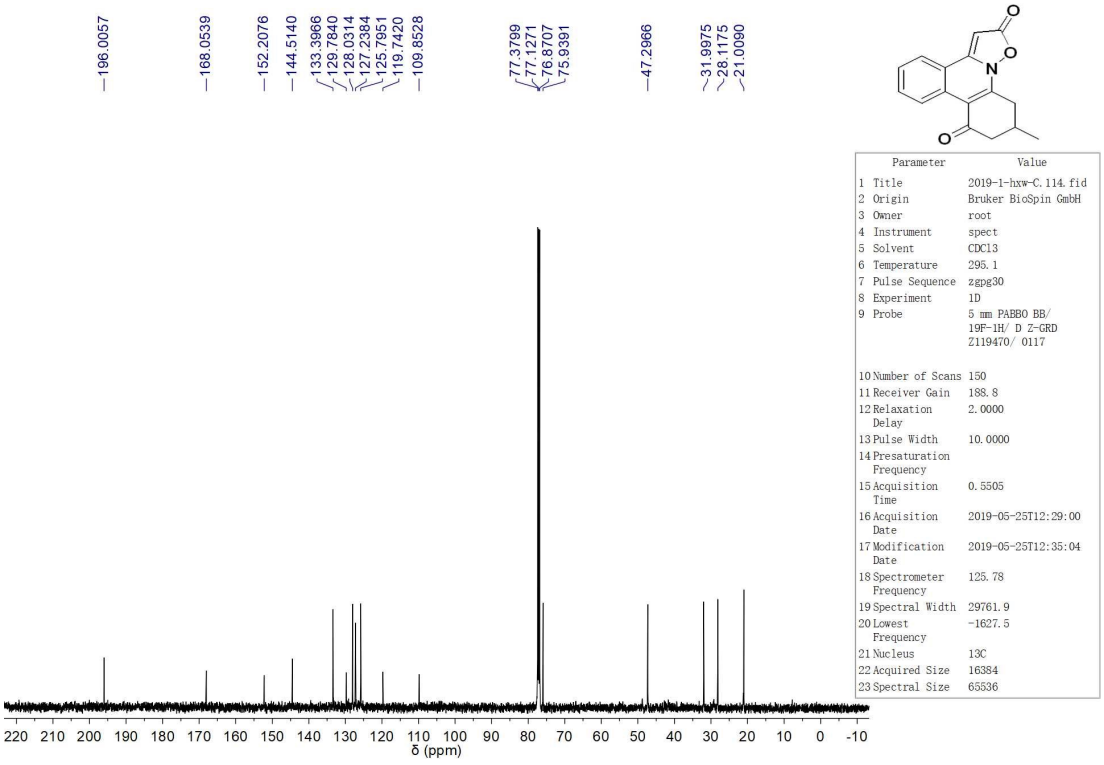

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.191.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.1 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 114.1 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-07-11T18:36:00 |
| 17 Modification Date | 2019-07-11T18:36:18 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1517.8 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



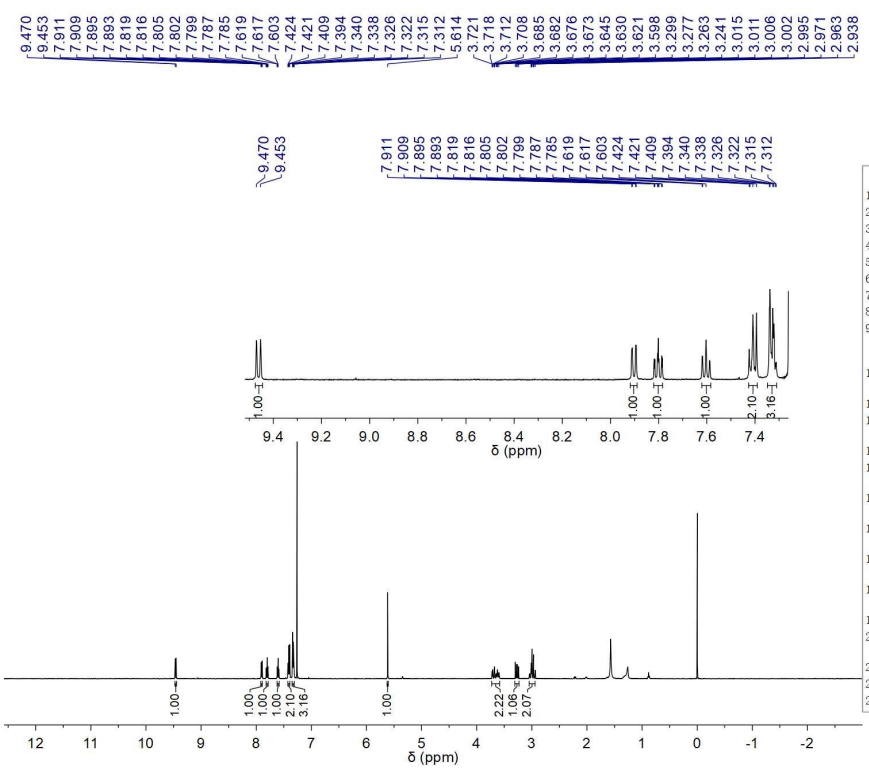

| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.171.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.2 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 1000 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-08-27T18:27:00 |
| 17 Modification Date | 2019-08-27T19:10:50 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

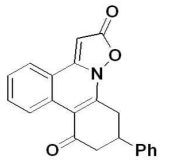
***10-Methyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (Table 2, compound 3ab)**



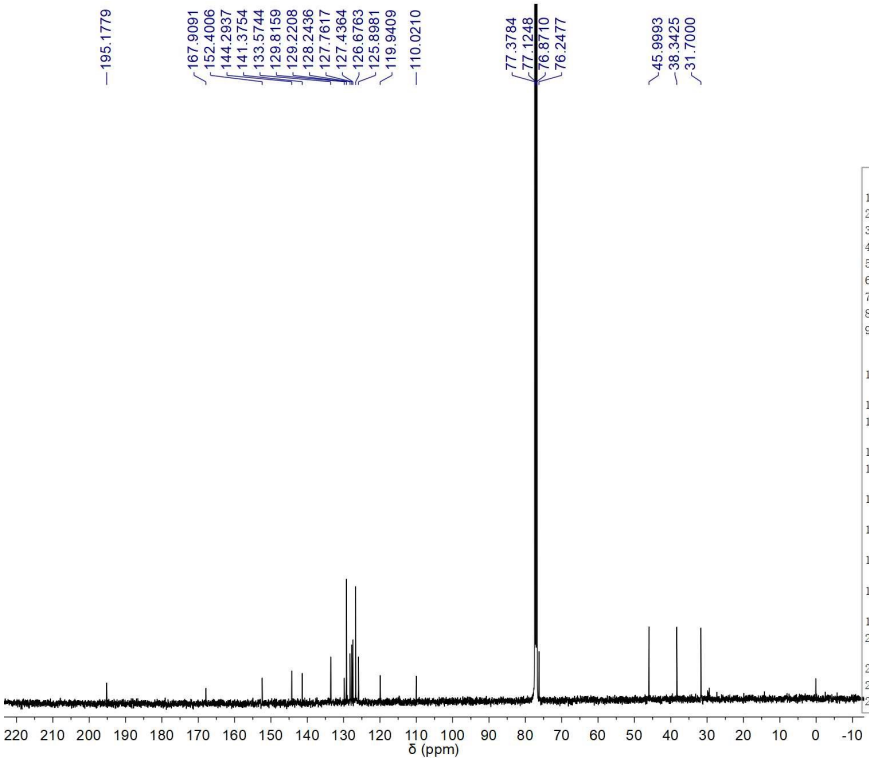



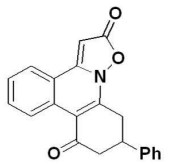
***10-Phenyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione* (Table 2, compound 3ac)**



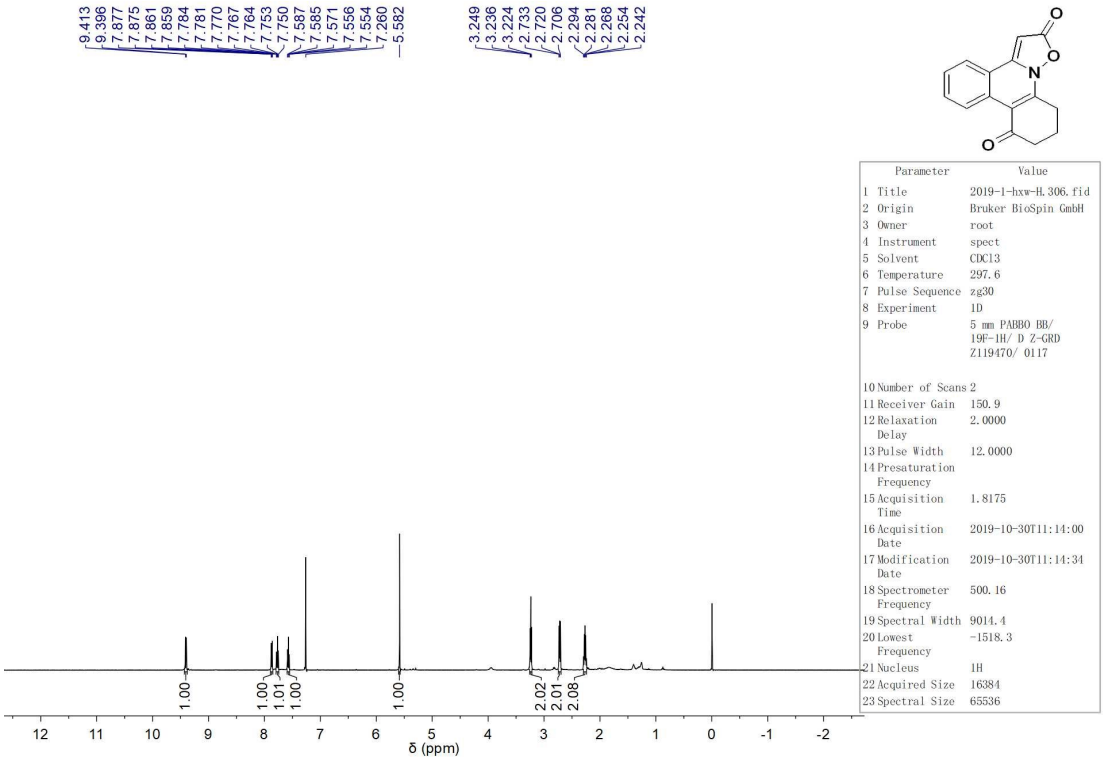
| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.319.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.8 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-11-12T11:27:16 |
| 17 Modification Date | 2019-11-12T11:27:18 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.8 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



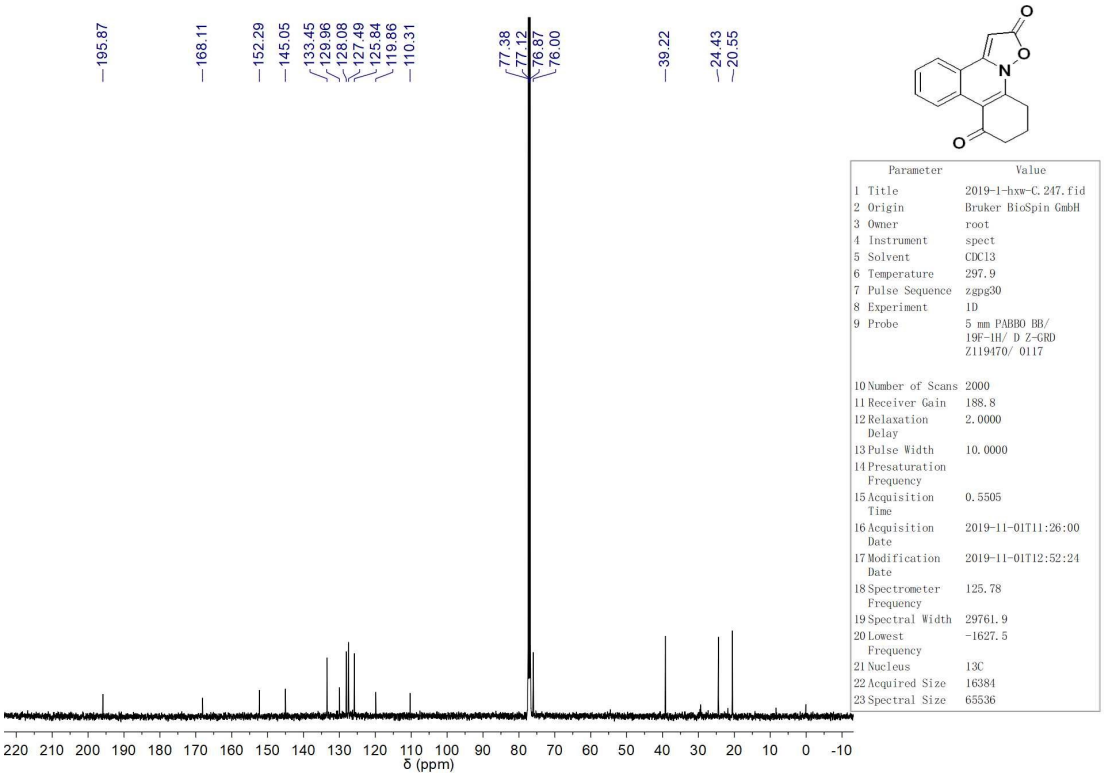



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.249.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 298.3 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 3000 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-11-12T14:03:31 |
| 17 Modification Date | 2019-11-12T14:03:34 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***10,11-Dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione*** **(Table 2, compound 3ad)**

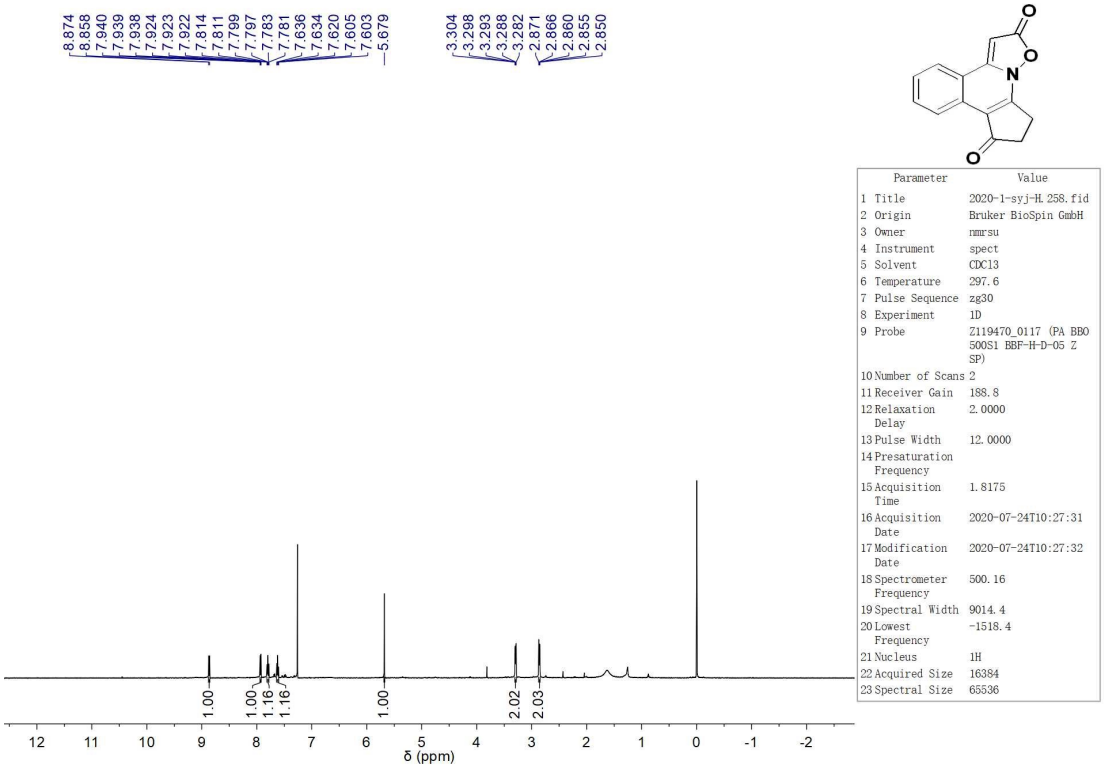



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-H.306.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.6 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 150.9 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2019-10-30T11:14:00 |
| 17 Modification Date | 2019-10-30T11:14:34 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.3 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

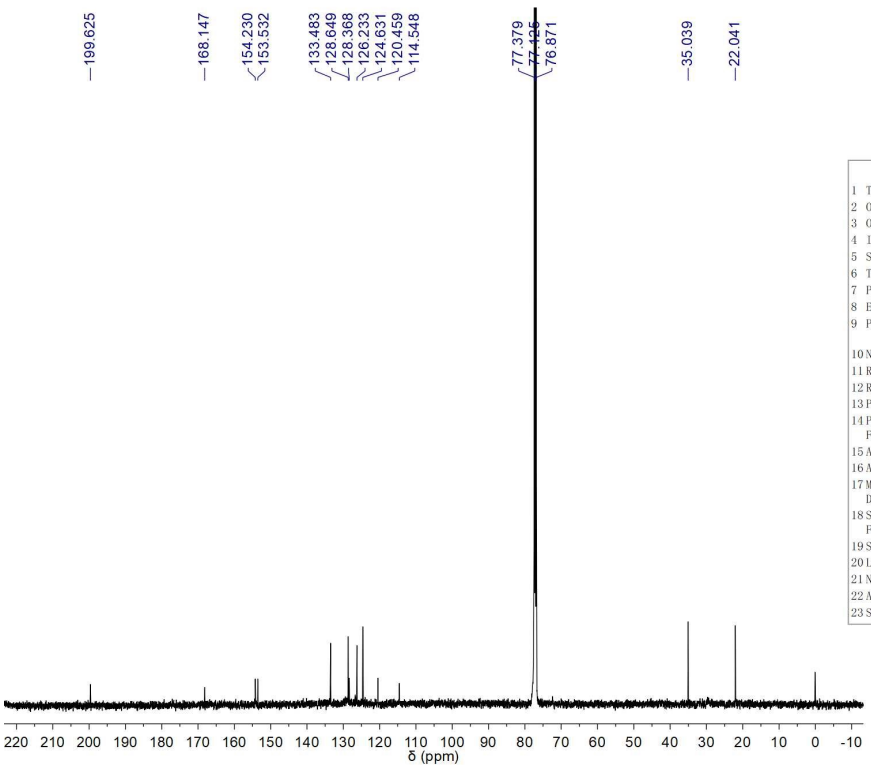



| Parameter | Value |
|---|---|
| 1 Title | 2019-1-hxw-C.247.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | root |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.9 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117 |
| 10 Number of Scans | 2000 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2019-11-01T11:26:00 |
| 17 Modification Date | 2019-11-01T12:52:24 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***9,10-Dihydrocyclopenta[c]isoxazolo[3,2-a]isoquinoline-2,8-dione*** **(Table 2, compound 3ae)**

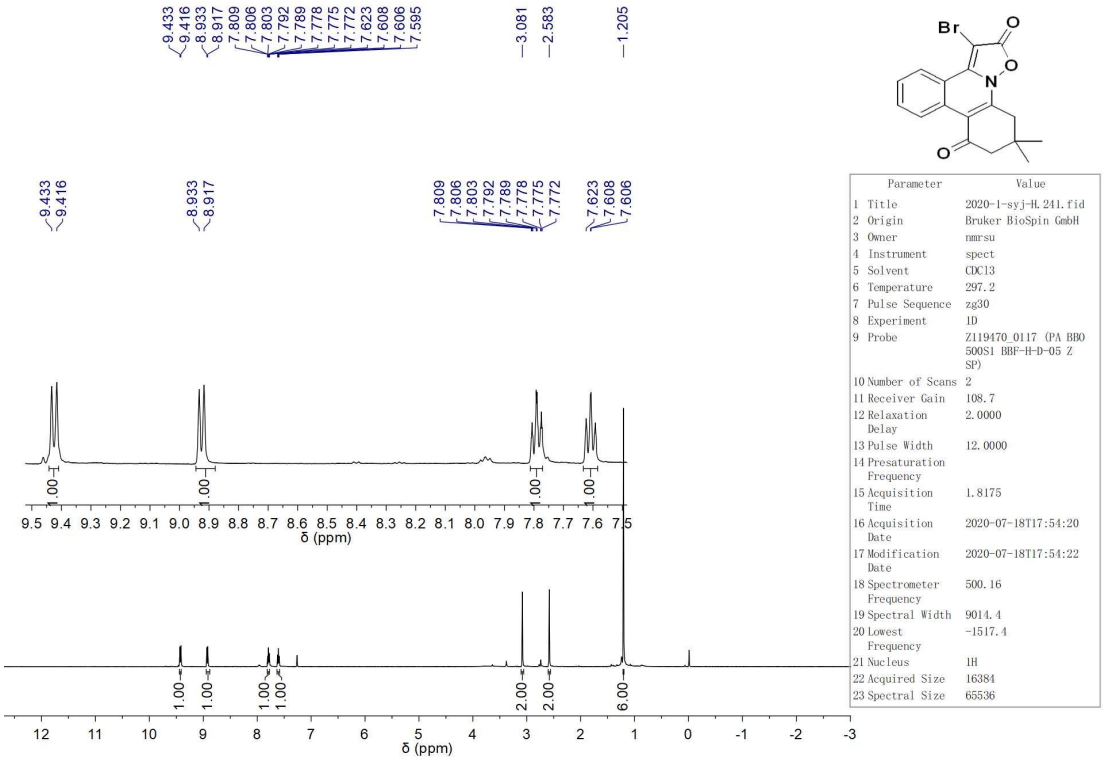



| Parameter | Value |
|---|---|
| 1 Title | 2020-1-syj-H.258.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | nmrsu |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.6 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2020-07-24T10:27:31 |
| 17 Modification Date | 2020-07-24T10:27:32 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1518.4 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |



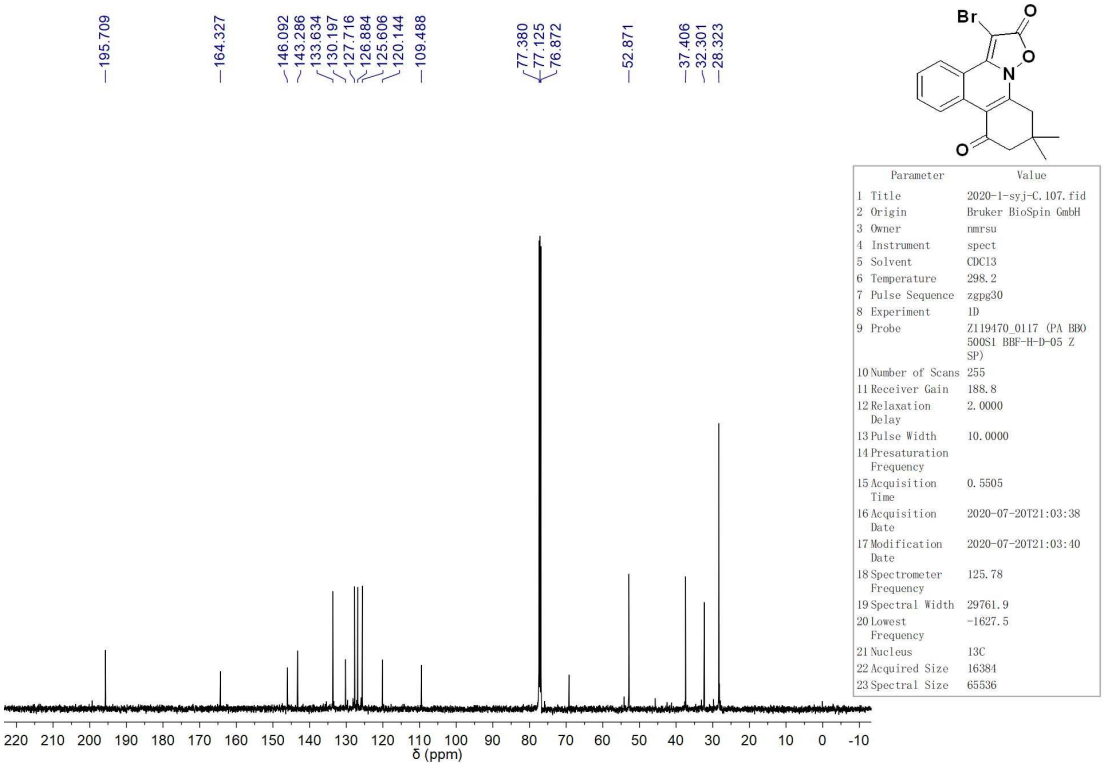

| Parameter | Value |
|---|---|
| 1 Title | 2020-1-syj-C.110.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | nmrsu |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.9 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 3800 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2020-07-26T14:40:12 |
| 17 Modification Date | 2020-07-26T14:40:14 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |

***3-Bromo-10,10-dimethyl-10,11-dihydro-2H-isoxazolo[2,3-f]phenanthridine-2,8(9H)-dione***
**(Scheme 2, compound 4)**






| Parameter | Value |
|---|---|
| 1 Title | 2020-1-syj-H 241.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | nmrsu |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 297.2 |
| 7 Pulse Sequence | zg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 2 |
| 11 Receiver Gain | 108.7 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 12.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 1.8175 |
| 16 Acquisition Date | 2020-07-18T17:54:20 |
| 17 Modification Date | 2020-07-18T17:54:22 |
| 18 Spectrometer Frequency | 500.16 |
| 19 Spectral Width | 9014.4 |
| 20 Lowest Frequency | -1517.4 |
| 21 Nucleus | 1H |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |






| Parameter | Value |
|---|---|
| 1 Title | 2020-1-syj-C.107.fid |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Owner | nmrsu |
| 4 Instrument | spect |
| 5 Solvent | CDCl3 |
| 6 Temperature | 298.2 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
| 9 Probe | Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP) |
| 10 Number of Scans | 255 |
| 11 Receiver Gain | 188.8 |
| 12 Relaxation Delay | 2.0000 |
| 13 Pulse Width | 10.0000 |
| 14 Presaturation Frequency | |
| 15 Acquisition Time | 0.5505 |
| 16 Acquisition Date | 2020-07-20T21:03:38 |
| 17 Modification Date | 2020-07-20T21:03:40 |
| 18 Spectrometer Frequency | 125.78 |
| 19 Spectral Width | 29761.9 |
| 20 Lowest Frequency | -1627.5 |
| 21 Nucleus | 13C |
| 22 Acquired Size | 16384 |
| 23 Spectral Size | 65536 |